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FILE COVERS 1907 - 5 Nov 2007  VOL 147 ISS 20
FILE LAST UPDATED: 4 Nov 2007  (20071104/ED)
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Compounds associated with the pre grant publication of instant application:

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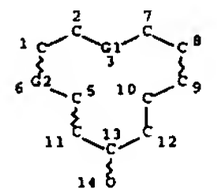

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
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                 C14/ESS OR C15/ESS OR C16/ESS
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L13           27 SEA FILE=CAPLUS ABB=ON  PLU=ON  L12

=> d l13 ibib abs hitstr 1-27

L13  ANSWER 1 OF 27  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2007:582533  CAPLUS  Full-text
DOCUMENT NUMBER:          147:211639
TITLE:                    Synthesis of migrastatin and its macrolide core
AUTHOR(S):                Reymond, Sebastien; Cossy, Janine
CORPORATE SOURCE:         Laboratoire de Chimie Organique associe au CNRS,
                          ESPCI, Paris, 75231, Fr.
SOURCE:                   Tetrahedron (2007), 63(26), 5918-5929
                          CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER:                Elsevier Ltd.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 147:211639
GI
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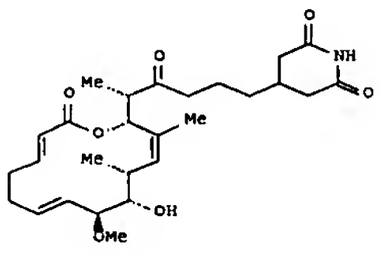

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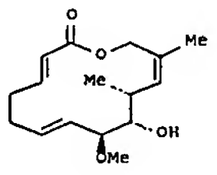

II

AB Migrastatin (I) and its macrolactone subunit II are potent antimetastatic agents. Both were synthesized by using a ring-closing metathesis (RCM) to establish the macrolactone core, and the control of the (Z)-trisubstituted double bond at C11-C12 was achieved by using a Still-Gennari olefination.

```
IT  545339-21-7P 663613-00-1P 663613-13-6P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
    (Reactant or reagent)
       (synthesis of migrastatin and its macrolide core via ring-closing
       metathesis, Still-Gennari olefination, and stereoselective
       crotylmetalation reactions)
RN  545339-21-7  CAPLUS
CN  2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-[[(1,1-
    dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-
    oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]-  (CA INDEX NAME)

Absolute stereochemistry.  Rotation (+).
Double bond geometry as shown.
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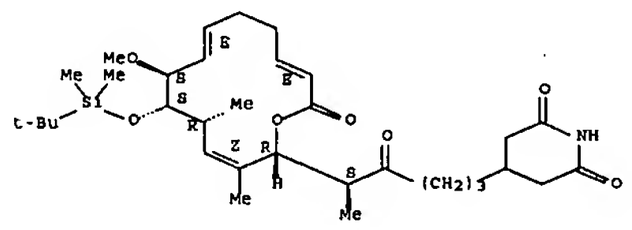

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RN  663613-00-1  CAPLUS
CN  Oxacyclotetradeca-3,7,12-trien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-
    , (3E,7E,9S,10S,11R,12Z)-  (CA INDEX NAME)

Absolute stereochemistry.  Rotation (+).
Double bond geometry as shown.
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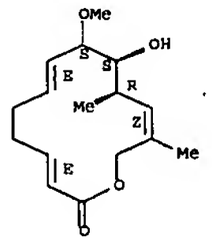

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RN  663613-13-6  CAPLUS
CN  Oxacyclotetradeca-3,7,12-trien-2-one, 10-[[(1,1-
    dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-,
    (3E,7E,9S,10S,11R,12Z)-  (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.
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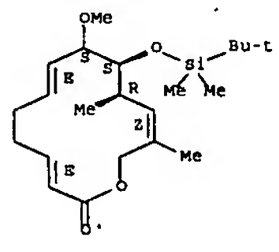

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IT  314245-65-3P, (+)-Migrastatin
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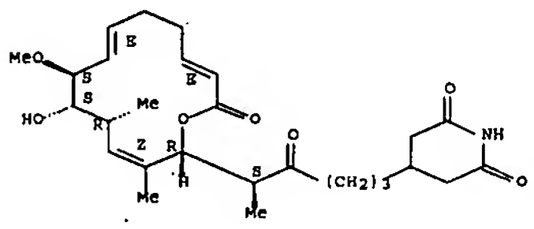
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of migrastatin and its macrolide core via ring-closing metathesis, Still-Gennari olefination, and stereoselective crotylmetalation reactions)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1313691 CAPLUS Full-text
DOCUMENT NUMBER: 146:266505
TITLE: Migrastatin acts as a muscarinic acetylcholine receptor antagonist
AUTHOR(S): Nakae, Koichi; Nishimura, Yoshio; Ohba, Syunichi; Akamatsu, Yuzuru
CORPORATE SOURCE: Bioactive Molecules Research Group, Microbial Chemistry Research Center, 3-14-23 Kamiosaki, Shinagawa-ku, Tokyo, 141-0021, Japan
SOURCE: Journal of Antibiotics (2006), 59(11), 685-692
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:266505

AB Migrastatin and its analogs have various biol. activities such as inhibition of cell migration and anchorage-independent growth of cancer cells. Although its biosynthesis and chemical synthesis have been under investigation, little is known about the biol. target of migrastatin. Here, we found that migrastatin inhibited intracellular calcium mobilization induced by carbachol in neuroblastoma SK-N-SH cells without affecting Ca2+ mobilization and cAMP accumulation induced by ligands of other receptors. The binding of [3H] N-methyl-scopolamine, an antagonist for muscarinic receptor was also inhibited by migrastain. Functionally, migrastatin inhibited Ca2+ mobilization induced by carbachol in primary cultures of smooth muscle cells of rat bladder. This study reveals that migrastatin acts as a muscarinic acetylcholine receptor antagonist.

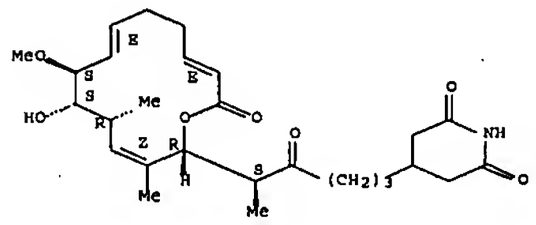
IT 314245-65-3, Migrastatin
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); RCT

(Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(migrastatin acts as muscarinic receptor antagonist)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1221342 CAPLUS Full-text
DOCUMENT NUMBER: 146:142401
TITLE: Total synthesis of (+)-migrastatin
AUTHOR(S): Reymond, Sebastien; Cossy, Janine
CORPORATE SOURCE: Laboratoire de Chim. Org., UMR CNRS 7084, Paris, 75231, Fr.
SOURCE: European Journal of Organic Chemistry (2006), (21), 4800-4804
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:142401

AB (+)-Migrastatin, an antimetastatic agent, was synthesized by using three ruthenium-catalyzed metathesis reactions: a ring-closing metathesis (RCM) to control the (Z)-trisubstituted double bond at C11-C12, another RCM at C6-C7 to establish the macro lactone core, and a cross-metathesis to install the glutarimide side chain at C16-C17. The stereogenic centers at C9, C10, C13, and C14 were introduced by using two stereoselective crotylmetalations.

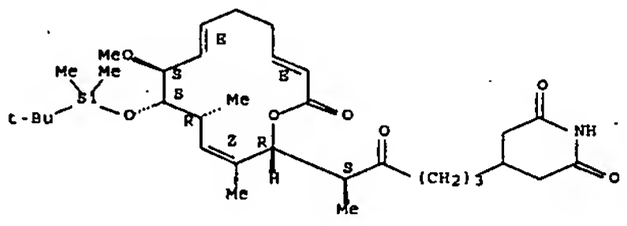
IT 545339-21-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of migrastatin via ring-closing metathesis, cross-metathesis and stereoselective crotylmetalation)

RN 545339-21-7 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

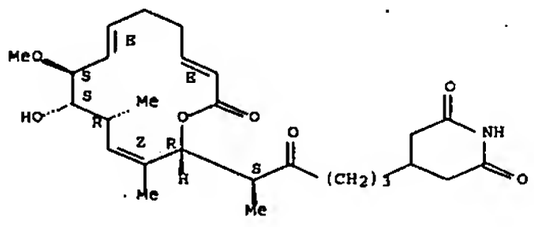


IT 314245-65-3P, (+)-Migrastatin
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of migrastatin via ring-closing metathesis, cross-metathesis and stereoselective crotylmetalation)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1191620 CAPLUS Full-text
DOCUMENT NUMBER: 146:121724
TITLE: Thermolysis of Isomigrastatin and Its Congeners via [3,3]-Sigmatropic Rearrangement: A New Route to the Synthesis of Migrastatin and Its Analogues
AUTHOR(S): Ju, Jianhua; Lim, Si-Kyu; Jiang, Hui; Seo, Jeong-Woo; Her, Yeng; Shen, Ben
CORPORATE SOURCE: Division of Pharmaceutical Sciences, University of Wisconsin National Cooperative Drug Discovery Group and Department of Chemistry, University of Wisconsin-Madison, Madison, WI, 53705, USA
SOURCE: Organic Letters (2006), 8(25), 5865-5868
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:121724
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

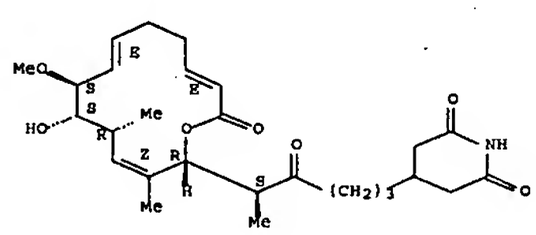
AB Thermolysis of isomigrastatin (I) under neat heating conditions afforded migrastatin (II). The reaction is proposed to proceed via a concerted [3,3]-sigmatropic rearrangement by which ring expansion is achieved regio- and enantiospecifically. The general applicability of this reaction was demonstrated with six addnl. isomigrastatin congeners, providing a new route to the synthesis of migrastatin analogs.

IT 314245-65-3P, Migrastatin
RL: SPN (Synthetic preparation); PREP (Preparation)
(thermolysis of isomigrastatin and congeners via [3,3]-sigmatropic rearrangement to give migrastatin and analogs)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:980081 CAPLUS Full-text
DOCUMENT NUMBER: 145:354863
TITLE: Glutarimide-containing polyketide analogs and their synthesis
INVENTOR(S): Shen, Ben
PATENT ASSIGNEE(S): Wisconsin Alumni Research Foundation, USA
SOURCE: U.S. Pat. Appl. Publ., 54pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006211736	A1	20060921	US 2006-275556	20060113
PRIORITY APPLN. INFO.:			US 2005-593434P P	20050113

OTHER SOURCE(S): CASREACT 145:354863; MARPAT 145:354863

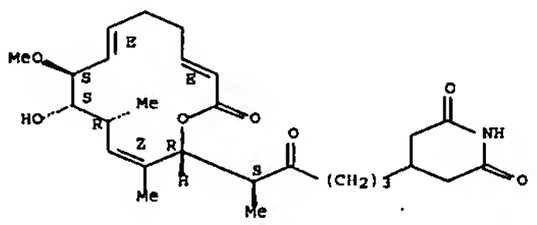
AB The present invention provides library of glutarimide-containing polyketide analogs, such as analogs of migrastatin, iso-migrastatin, dorrigocin A and B, epi-dorrigocin, NK30424 A and B and lactimidomycin, methods of synthesizing and using these analogs and further methods of creating a combinatorial library of these compds. through chemical modifications.

IT 314245-65-3P, Migrastatin
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(glutarimide-containing polyketide analogs and methods for their synthesis)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



L13 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	2006:846578 CAPLUS Full-text
DOCUMENT NUMBER:	145:284394
TITLE:	Suppression of multidrug resistance by migrastatin
AUTHOR(S):	Takemoto, Yasushi; Tashiro, Etsu; Imoto, Masaya
CORPORATE SOURCE:	Department of Biosciences and Informatics, Faculty of Science and Technology, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama, 223-8522, Japan
SOURCE:	Journal of Antibiotics (2006), 59(7), 435-438 CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER:	Japan Antibiotics Research Association
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB Migrastatin (MGS) is a Streptomyces metabolite that inhibits cancer cell migration. In this study, we found that MGS also enhanced the cytotoxicity of vinblastine, vincristine, and taxol in P-glycoprotein-overexpressing VJ-300 cells and P388/VCR cells. Furthermore, MGS increased the intracellular concentration of labeled vinblastine, vincristine, and taxol in both VJ-300 cells and P388/VCR cells. P-glycoprotein was photolabeled with [3H]azidopine, but this photolabeling was significantly inhibited in the presence of MGS.

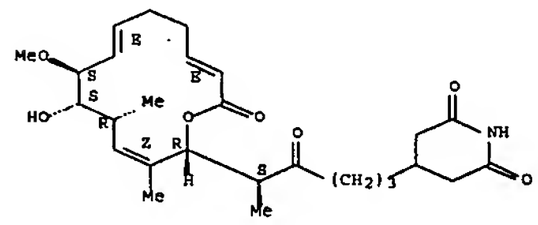
These results indicated that MGS directly interacts with and inhibits P-glycoprotein, thereby sensitizing drug-resistant cells to anticancer drugs.

IT 314245-65-3, Migrastatin
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(suppression of multidrug resistance by migrastatin)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	2006:757582 CAPLUS Full-text
DOCUMENT NUMBER:	145:356540
TITLE:	A convergent synthesis of the macrolide core of migrastatin
AUTHOR(S):	Baba, V. Sai; Das, Parthasarathi; Mukkanti, K.; Iqbal, Javed
CORPORATE SOURCE:	Discovery Research, Dr. Reddy's Laboratories Ltd., Hyderabad, 500 049, India
SOURCE:	Tetrahedron Letters (2006), 47(34), 6083-6086 CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER:	Elsevier B.V.
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 145:356540

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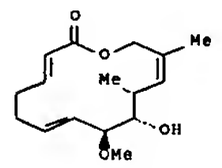

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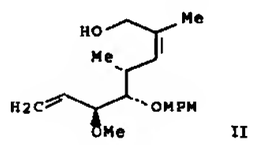


II

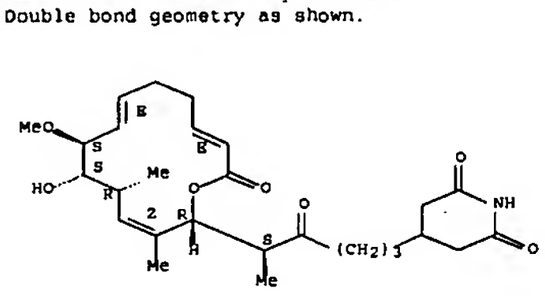
AB We describe an efficient synthesis of the 14-membered macrolide core I of migrastatin via key intermediate II employing a diastereoselective aldol condensation, Lewis acid mediated diastereoselective addition and an exclusive (Z)-olefination sequence. Yamaguchi esterification of the key intermediate II followed by ring-closing metathesis (RCM) produced macrolide I with high selectivity and good yield.

IT 314245-65-3, Migrastatin
RL: PNU (Preparation, unclassified)
(synthesis of the macrolide core of migrastatin via (Z)-olefination, Yamaguchi esterification and ring-closing metathesis)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

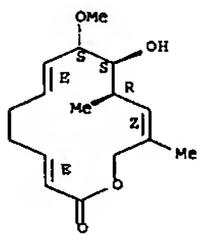


IT 663613-00-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of the macrolide core of migrastatin via (Z)-olefination, Yamaguchi esterification and ring-closing metathesis)

RN 663613-00-1 CAPLUS

CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

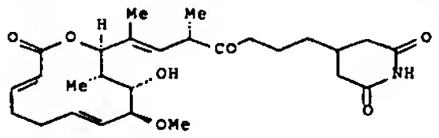
L13 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	2006:333580 CAPLUS Full-text
DOCUMENT NUMBER:	144:350443
TITLE:	Synthesis of isomigrastatin analogs for use in pharmaceutical compositions for the treatment of cancer and as angiogenesis inhibitors
INVENTOR(S):	Danishefsky, Samuel J.; Mandal, Mihirbaran; Dorn, David C.; Moore, Malcolm A. S.
PATENT ASSIGNEE(S):	Sloan-Kettering Institute for Cancer Research, USA
SOURCE:	PCT Int. Appl., 149 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006034478	A2	20060330	WO 2005-US34305	20050923
WO 2006034478	A3	20061130		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
WO 2006001967	A2	20060105	WO 2005-US18603	20050525
WO 2006001967	A3	20060727		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
CA 2582766	A1	20060330	CA 2005-2582766	20050923
EP 1805161	A2	20070711	EP 2005-800816	20050923
PRIORITY APPLN. INFO.:			US 2004-612415P P	20040923
			WO 2005-US18603 A	20050525
			US 2004-574114P P	20040525
			WO 2005-US34305 W	20050923

OTHER SOURCE(S): MARPAT 144:350443

GI



I

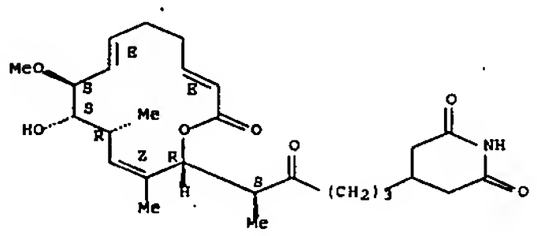
AB Isomigrastatin (I) and its macrolide analogs were synthesized via multistep macrocyclization synthetic sequences which included ring-closing metathesis reactions for therapeutic use in the treatment of various disorders including cancer, metastasis and disorders involving increased angiogenesis. The angiogenesis dependent diseases treatable by theses isomigrastatinn analogs include ocular angiogenic diseases, diabetic retinopathy, retinopathy of prematurity, corneal graft rejection, neovascular glaucoma, retrolental fibroplasias, rubeosis, solid tumors, blood born tumors, leukemia, tumor metastases, benign tumors, acoustic neuromas, neurofibromas, trachomas, pyogenic granulomas, rheumatoid arthritis, psoriasis, Osler-Webber Syndrome, myocardial angiogenesis, plaque neovascularization, telangiectasia, hemophiliac joints, angiofibroma, or wound granulation. Also, these isomigrastatin analogs, alone or in combination with other anti-cancer agents, were claimed for use inhibiting metastasis of tumors of the prostate, breast, colon, bladder, cervical, skin, testicular, kidney, ovarian, stomach, brain, liver, pancreatic or esophageal cancer or lymphoma, leukemia, or multiple myeloma.

IT 314245-65-3DP, analogs
RL: PAC (Pharmacological activity); PNU (Preparation, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of isomigrastatin analogs for use in pharmaceutical compns. for treatment of cancer and as angiogenesis inhibitors)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



L13 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:316673 CAPLUS Full-text

DOCUMENT NUMBER: 144:346441
TITLE: Method for synthesizing derivatives of organic compound produced by microorganism, compound library, its preparation method, and screening method
INVENTOR(S): Imoto, Masaya; Ohta, Hiromichi; Miyamoto, Kenji
PATENT ASSIGNEE(S): Keio University, Japan
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006035770	A1	20060406	WO 2005-JP17745	20050927
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
JP 2006087392	A	20060406	JP 2004-279597	20040927
JP 3916166	B2	20070516		
CA 2581254	A1	20060406	CA 2005-2581254	20050927
EP 1795603	A1	20070613	EP 2005-788164	20050927
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 101027405	A	20070829	CN 2005-80032311	20050927

PRIORITY APPLN. INFO.:
JP 2004-279597 A 20040927
WO 2005-JP17745 W 20050927

AB A method for synthesizing derivs. of a natural compound, a method for preparing a compound library containing the natural compound derivs., a compound library containing the natural compound derivs. as well as a screening method using the compound library are provided, which are useful in random high-throughput screening (HTS), search for a drugs or agricultural chemical, search for a lead compound for a drug or agricultural chemical, or else. The method for synthesizing derivs. of a natural compound comprises culturing microorganism (e.g., archaebacterium, eubacteria, protist, fungi, Ascomycetes, Zygomycetes, Basidiomycetes, Deuteromycetes, Myxomycetes, cellular Myxomycetes, Actinomyces) capable of producing an organic compound in a specified culture medium, and reacting the organic compound obtained by the culture with a reagent (e.g., reaction reagents for oxidation, reduction, epoxidn., dihydroxylation, oxidative cleavage, hydrogen addition, etherification, halogenation, nitration, sulfonation, diazotization, aldol reaction, alkylation) capable of synthesizing a derivative of the organic compound in the culture medium. By creating a library containing the derivs. thus obtained, enabled are random HTS, the search for a drug or agricultural chemical, the search for a lead compound of drugs or agricultural chems., and so on.

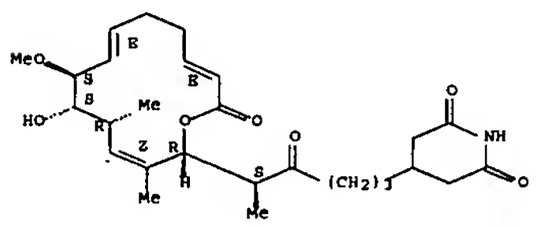
IT 314245-65-3P
RL: BPN (Biosynthetic preparation); CRT (Combinatorial reactant); RCT (Reactant); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)

(method for synthesizing derivs. of organic compound produced by microorganism, and method for preparing compound library for drug screening)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

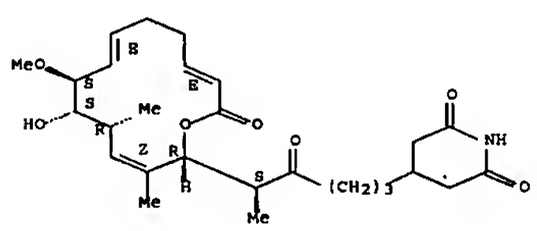


IT 314245-65-3DP, derivative
RL: BSU (Biological study, unclassified); CPN (Combinatorial preparation); CST (Combinatorial study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation)
(method for synthesizing derivs. of organic compound produced by microorganism, and method for preparing compound library for drug screening)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

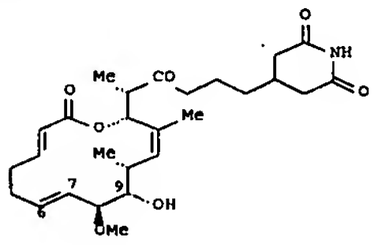
L13 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:10861 CAPLUS Full-text

DOCUMENT NUMBER: 144:88082
TITLE: Preparation of migrastatin and its analogs for use in pharmaceutical compositions for the treatment of cancer
INVENTOR(S): Danishefsky, Samuel J.; Gaul, Christoph; Njardarson, Jon T.; Moore, Malcolm A. S.; Wu, Kaida; Dorn, David C.; Mandal, Mihirbaran
PATENT ASSIGNEE(S): Sloan-Kettering Institute for Cancer Research, USA
SOURCE: PCT Int. Appl., 266 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006001967	A2	20060105	WO 2005-US18603	20050525
WO 2006001967	A3	20060727		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
CA 2582766	A1	20060330	CA 2005-2582766	20050923
WO 2006034478	A2	20060330	WO 2005-US34305	20050923
WO 2006034478	A3	20061130		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1805161	A2	20070711	EP 2005-800816	20050923

PRIORITY APPLN. INFO.:
US 2004-574114P P 20040525
US 2004-612415P P 20040923
WO 2005-US18603 A 20050525
WO 2005-US34305 W 20050923

OTHER SOURCE(S): MARPAT 144:88082
GI



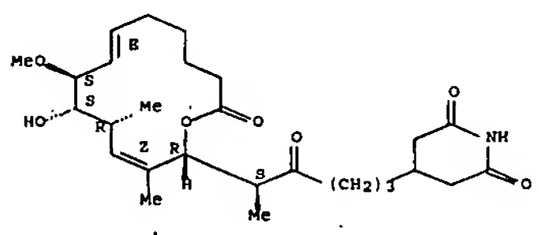
I

AB Migrastatin (I) and macrolide analogs thereof were prepared for therapeutic use in the treatment of cancer, particularly for inhibition of colon and/or ovarian tumor metastasis. A ring-closing metathesis reaction of a 6,7-divinyl-9-O-silyl-protected open-chain precursor was used to form the 6,7-olefinic bond, and thus, the core macrolide ring of I. I and some of its prepared analogs were assayed for anticancer activity against a number of human cancer cell lines, such as HT29 colon cancer cells and Ovcar3 ovarian cancer cells.

IT 663612-96-2P 663613-01-2P 663613-07-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of migrastatin and its analogs for use in pharmaceutical compns. for the treatment of cancer)

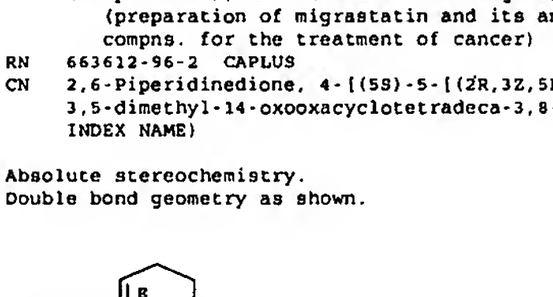
RN 663612-96-2 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 663613-01-2 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

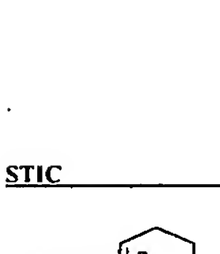


RN 663612-97-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]-1-methyl- (CA INDEX NAME)

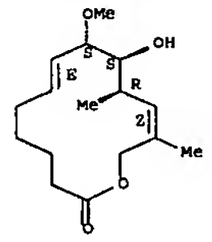
Absolute stereochemistry.
Double bond geometry as shown.

RN 663613-00-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

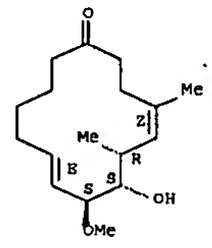


RN 663613-10-3 CAPLUS



RN 663613-07-8 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



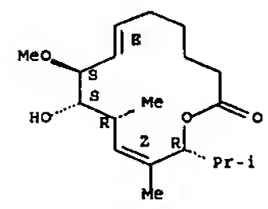
IT 314245-65-3P, (+)-Migrastatin 663612-97-3P
663613-00-1P 663613-10-3P 663613-11-4P
760900-67-3P 760900-69-9P 760900-84-9P
760988-86-1P 760989-88-3P 760989-89-4P
760989-90-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of migrastatin and its analogs for use in pharmaceutical compns. for the treatment of cancer)

RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

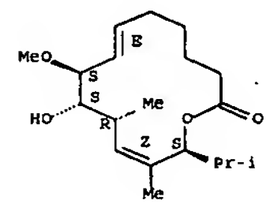
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-14-(1-methylethyl)-, (7E,9S,10S,11R,12Z,14R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



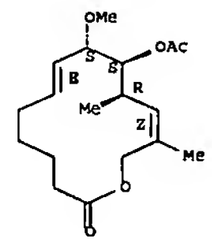
RN 663613-11-4 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-14-(1-methylethyl)-, (7E,9S,10S,11R,12Z,14S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



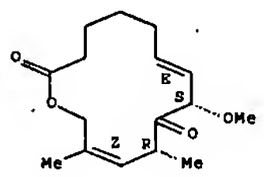
RN 760988-67-8 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-(acetyloxy)-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



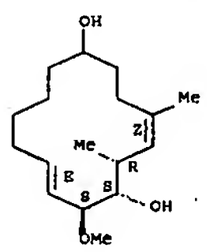
RN 760988-68-9 CAPLUS
CN Oxacyclotetradeca-7,12-diene-2,10-dione, 9-methoxy-11,13-dimethyl-, (7E,9S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



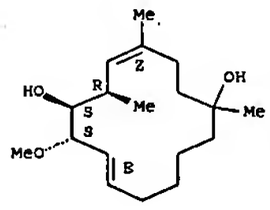
RN 760988-84-9 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4-dimethyl-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



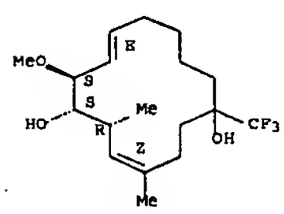
RN 760988-86-1 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4,7-trimethyl-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



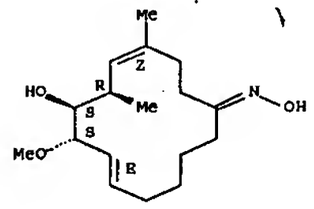
RN 760988-88-3 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4-dimethyl-7-(trifluoromethyl)-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 760988-89-4 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, oxime, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

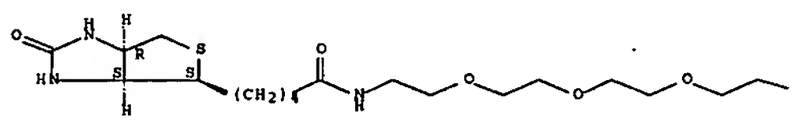
Absolute stereochemistry.
Double bond geometry as described by E or Z.



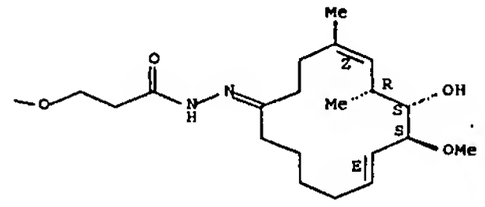
RN 760988-90-7 CAPLUS
CN 4,7,10,13-Tetraoxa-16-azaheneicosanoic acid, 21-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-17-oxo-, [(4Z,6R,7S,8S,9E)-7-hydroxy-8-methoxy-4,6-dimethyl-4,9-cyclotetradecadien-1-ylidene]hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.

PAGE 1-A

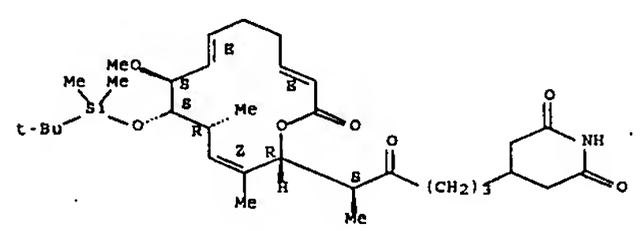


PAGE 1-B



IT 545339-21-7P 663613-13-6P 663613-14-7P
663613-16-9P 760988-66-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of migrastatin and its analogs for use in pharmaceutical compns. for the treatment of cancer)
RN 545339-21-7 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-13-6 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

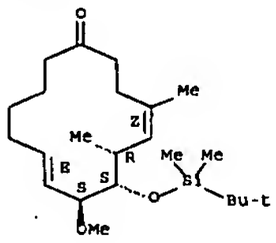
Absolute stereochemistry.
Double bond geometry as shown.

RN 663613-14-7 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

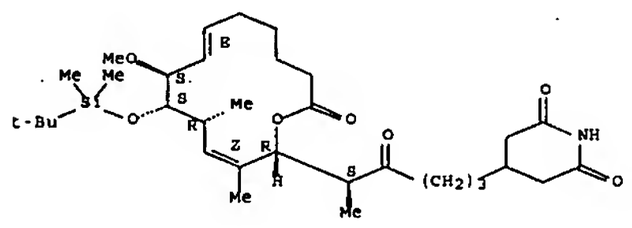
RN 663613-16-9 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



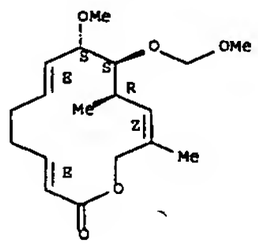
RN 760988-66-7 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



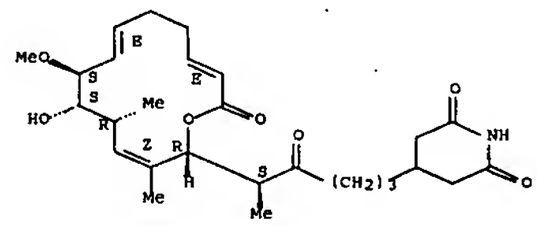
IT 494834-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of migrastatin and its analogs for use in pharmaceutical compns. for the treatment of cancer)
RN 494834-82-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 9-methoxy-10-(methoxymethoxy)-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L13 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:704284 CAPLUS Full-text
DOCUMENT NUMBER: 143:385219
TITLE: Iso-Migrastatin Congeners from Streptomyces platensis and Generation of a Glutarimide Polyketide Library Featuring the Dorrigocin, Lactimidomycin, Migrastatin, and NK30424 Scaffolds
AUTHOR(S): Ju, Jianhua; Lim, Si-Kyu; Jiang, Hui; Seo, Jeong-Woo; Shen, Ben
CORPORATE SOURCE: Division of Pharmaceutical Sciences and Department of Chemistry, University of Wisconsin Madison, Madison, WI, 53705, USA
SOURCE: Journal of the American Chemical Society (2005), 127(34), 11930-11931
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Iso-Migrastatin (10) has been shown to be the main natural product of Streptomyces platensis, which undergoes a facile, H2O-mediated rearrangement into dorrigocin A (2), 13-epi-dorrigocin A (11), dorrigocin B (3), and migrastatin (1). Eight new congeners (12-19) of 10 were characterized. They can undergo the same H2O-mediated rearrangement into the corresponding 1, 2, 3, and 11 analogs (20-43) or 1,4-Michael addition with cysteine to afford the corresponding analogs (44-51) of NK30424 A and B (5, 6). This study generated a 47-member library of glutarimide polyketides, setting the stage to investigate the SAR for this family of natural products. These results also established the absolute stereochem. of 5 and 6 and shed new light into the post-polyketide synthase steps for 10 biosynthesis.
IT 314245-65-3
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(iso-Migrastatin congeners from Streptomyces platensis and generation of glutarimide polyketide library featuring the dorrigocin, lactimidomycin, Migrastatin, and NK30424 scaffolds)
RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

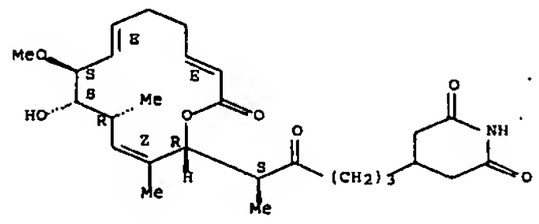
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

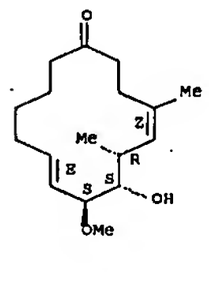
L13 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:247346 CAPLUS Full-text
DOCUMENT NUMBER: 142:403680
TITLE: Synthetic analogues of migrastatin that inhibit mammary tumor metastasis in mice
AUTHOR(S): Shan, Dandan; Chen, Lin; Njardarson, Jon T.; Gaul, Christoph; Ma, Xiaojing; Danishefsky, Samuel J.; Huang, Xin-Yun
CORPORATE SOURCE: Department of Physiology, Weill Medical College of Cornell University, New York, NY, 10021, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2005), 102(10), 3772-3776
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Tumor metastasis is the most common cause of death in cancer patients. Here, the authors show that two, fully synthetic migrastatin analogs, core. macroketone and core macrolactam, are potent inhibitors of metastasis in a murine breast tumor model. Administration of these readily accessible compds. nearly completely inhibits lung metastasis of highly metastatic mammary carcinoma cells. Treatment of tumor cells with core macroketone and core macrolactam blocks Rac activation, lamellipodia formation, and cell migration, suggesting that these chemical compds. interfere with the invasion step of the metastatic process. These compds. also inhibit the migration of human metastatic breast cancer cells, prostate cancer cells, and colon cancer cells but not normal mammary-gland epithelial cells, fibroblasts, and leukocytes. These data demonstrate that the macroketone and macrolactam core structures are specific small-mol. inhibitors of tumor metastasis. These compds. or their analogs could potentially be used in cancer-therapy strategies.
IT 314245-65-3, Migrastatin 663613-07-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(synthetic analogs of migrastatin that inhibit mammary tumor metastasis in mice)
RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-07-8 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



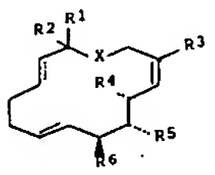
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:182633 CAPLUS Full-text
DOCUMENT NUMBER: 142:279984
TITLE: Preparation of migrastatin analogs as cell migration inhibitors
INVENTOR(S): Huang, Xin-Yun
PATENT ASSIGNEE(S): Cornell Research Foundation, Inc., USA
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005019181	A1	20050303	WO 2004-US9211	20040325

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-496165P P 20030819
OTHER SOURCE(S): CASREACT 142:279984; MARPAT 142:279984
GI



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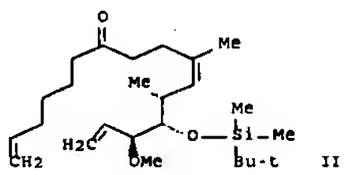
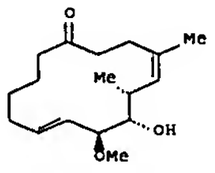


II



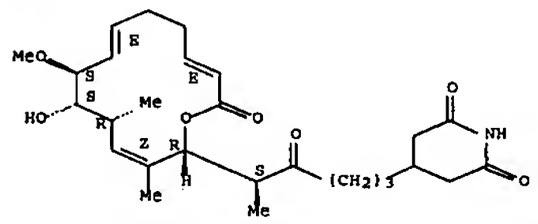
III

AB The present invention provides pharmaceutical compns. comprising a therapeutically effective amount of a migrastatin analogs, such as I [X = CH, N, NH, O; R1 = OH, CZ3; R1R2 = O; Z = halo; R3, R4 = H, alkyl; R5 = OH; R6 = alkyloxy; dashed bond = single or double bond], or a pharmaceutically acceptable salts thereof, for inhibiting cell migration. These compns. and methods can be used to inhibit metastasis of tumor cells in mammals. I are prepared via a ring-closing metathesis reaction. For example, tetraene II was prepared and treated with Grubbs' catalyst to give macrocyclic compound III after desilylation. In the group treated with 10 mg/kg of III, there were 3875 ± 2525 colonies (.apprx.94% inhibition of lung metastasis). The prepared migrastatin analogs were assayed as cell migration inhibitors [IC50 = 100 nM for III (4T1 tumor cells)].

IT 314245-65-3P, Migrastatin 663612-96-2P, 2,3-Dihydro-migrastatin 663612-97-3P, 2,3-Dihydro-N-methylmigrastatin 663613-00-1P 663613-01-2P 663613-07-8P 760988-88-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of migrastatin analogs as cell migration inhibitors for treating and preventing metastasis)

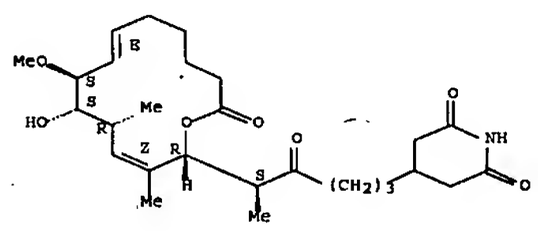
RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



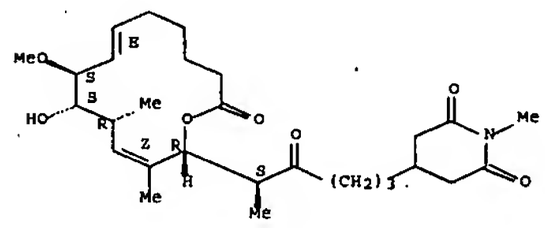
RN 663612-96-2 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



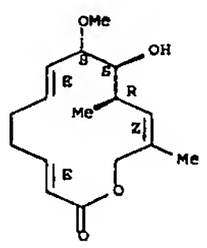
RN 663612-97-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]-1-methyl- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



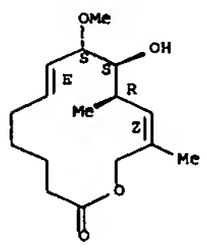
RN 663613-00-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



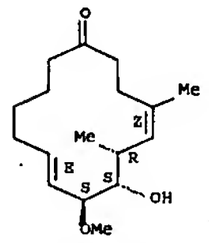
RN 663613-01-2 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



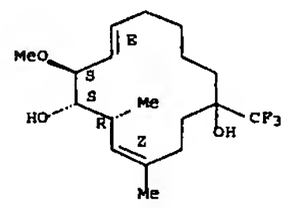
RN 663613-07-8 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 760988-88-3 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4-dimethyl-7-(trifluoromethyl)-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

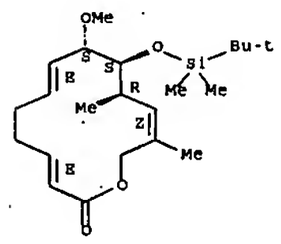
Absolute stereochemistry.
Double bond geometry as shown.



IT 663613-13-6P 663613-14-7P 663613-16-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of migrastatin analogs as cell migration inhibitors for treating and preventing metastasis)

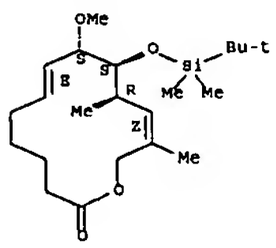
RN 663613-13-6 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



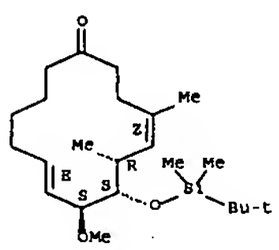
RN 663613-14-7 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 663613-16-9 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

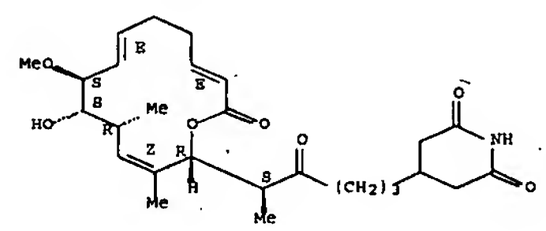
L13 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:64278 CAPLUS Full-text
DOCUMENT NUMBER: 142:312883
TITLE: Migrastatin and dorrigocins are shunt metabolites of iso-migrastatin
AUTHOR(S): Ju, Jianhua; Lim, Si-Kyu; Jiang, Hui; Shen, Ben
CORPORATE SOURCE: Division of Pharmaceutical Sciences and Department of Chemistry, University of Wisconsin Madison, Madison, WI, 53705, USA
SOURCE: Journal of the American Chemical Society (2005), 127(6), 1622-1623

CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Fermentation of Streptomyces platensis NRRL 18993 typically accumulated migrastatin (I), dorrigocin A (II) and B (III), and 13-epi-dorrigocin A (V). Supplement of XAD-16 resin to the fermentation, in contrast, resulted in exclusive production of iso-migrastatin (IV). In vitro studies showed that I, II, III, and V are stable in aqueous solution but IV undergoes rapid conversion into I, II, III, and V under the same condition. These results revealed that IV is the only bona fide natural product biosynthesized by S. platensis, and I, II, III, and V are shunt metabolites of IV. This study also established the stereochem. of II-V, with the exception of C-11 for III and IV. A mechanism for H2O-mediated regio- and stereospecific rearrangement of IV to I, II, III, and V is proposed and supported by incorporation of 18O from H218O.
IT 314245-65-3, Migrastatin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(migrastatin and dorrigocins are shunt metabolites of iso-migrastatin)
RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

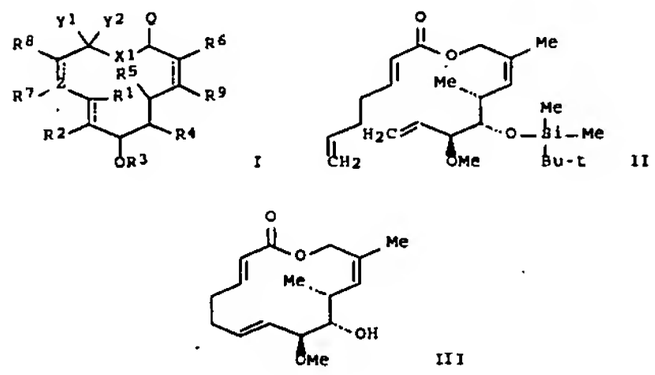
L13 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:857572 CAPLUS Full-text
DOCUMENT NUMBER: 141:331967
TITLE: Preparation of migrastatin analogs and their biological activity
INVENTOR(S): Danishefsky, Samuel J.; Gaul, Christoph; Njardarson, Jon T.
PATENT ASSIGNEE(S): Sloan-Kettering Institute for Cancer Research, USA

SOURCE: PCT Int. Appl., 254 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087673	A2	20041014	WO 2004-US9571	20040326
WO 2004087673	A3	20041104		
WO 2004087673	B1	20050310		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2520732	A1	20041014	CA 2004-2520732	20040326
EP 1613603	A2	20060111	EP 2004-758529	20040326
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
JP 2006521407	T	20060921	JP 2006-509430	20040326
US 2007037852	A1	20070215	US 2006-551158	20060925

PRIORITY APPLN. INFO.: US 2003-458827P P 20030328
US 2003-496165P P 20030819
WO 2004-US9571 W 20040326

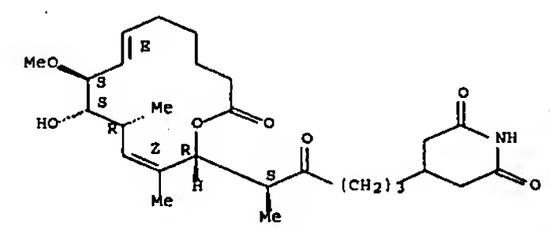
OTHER SOURCE(S): CASREACT 141:331967; MARPAT 141:331967
GI



I II III

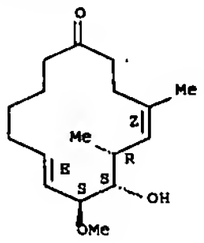
AB The present invention provides pharmaceutical compns. comprising a therapeutically effective amount of a compound of general formula I [R1, R2 = independently H, halide, cyano, NO2, etc.; R3 = H, alicyclic moiety, aryl, etc.; R4 = halide, OR10, NR10R11, R10, R11 = independently H, (hetero)aryl, alicyclic moiety, NR10R11 = heterocycle, heteroaryl; R5 = H, (hetero)aryl, (hetero)alicyclic, (hetero)aliphatic; R6 = H, halide, cyano, (hetero)aryl, amino, amido, etc.; R7, R8 = independently H, halide, cyano, amido, etc.; R7R8 = (hetero)aryl, (hetero)alicyclic; R9 = H, halide, cyano, sulfonyl, nitro, (hetero)aryl, etc.; R6R9 = (hetero)alicyclic, (hetero)aryl; Q = H, halide, cyano, sulfonyl, amido, etc.; X1 = O, S, amino, substituted carbon atom; Z = (CHRb)n, n = 1-5; Y1, Y2 = independently H, (hetero) aliphatic, (hetero)aryl, etc.], whereby the composition is formulated for administration to a subject to treat cancer, metastasis, and disorders involving increased angiogenesis. I are prepared via a ring-closing metathesis reaction. For example, tetraene II was prepared and treated with Grubbs' catalyst to give macrocyclic compound III after desilylation. III represents the core of migrastatin.
IT 663612-96-2P 663613-07-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of migrastatin and analogs for pharmaceutical compns. to treat wounds, inhibit angiogenesis, cell proliferation, cell migration, tumor metastasis, and the structure-activity relationship)
RN 663612-96-2 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



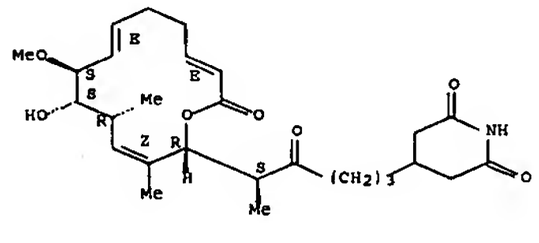
RN 663613-07-8 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



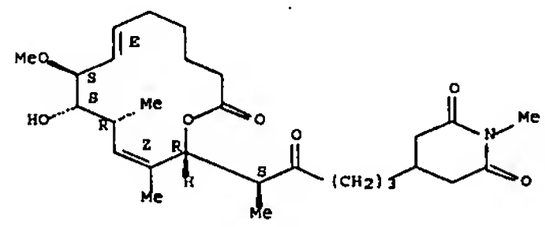
IT 314245-65-3P, Migrastatin 662612-97-3P
662612-00-1P 663613-01-2P 663613-10-3P
663613-11-4P 760988-67-8P 760988-68-9P
760988-84-9P 760988-86-1P 760988-88-3P
760988-89-4P 760988-90-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of migrastatin and analogs for pharmaceutical compns. to treat wounds, inhibit angiogenesis, cell proliferation, cell migration, tumor metastasis, and the structure-activity relationship)
RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



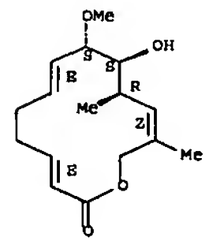
RN 663612-97-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]-1-methyl- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



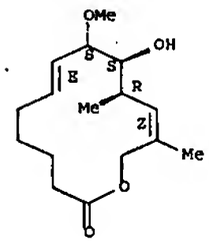
RN 663613-00-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-01-2 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

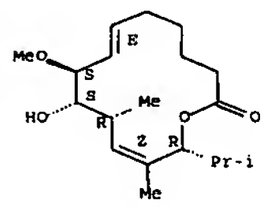
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-10-3 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-14-

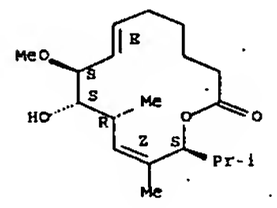
(1-methylethyl)-, (7E,9S,10S,11R,12Z,14R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



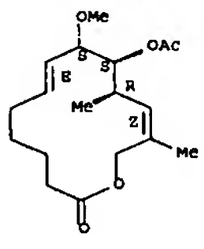
RN 663613-11-4 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-14-(1-methylethyl)-, (7E,9S,10S,11R,12Z,14S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



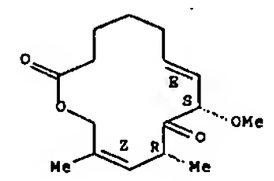
RN 760988-67-8 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-(acetyloxy)-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



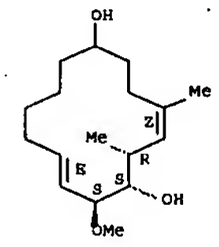
RN 760988-68-9 CAPLUS
CN Oxacyclotetradeca-7,12-diene-2,10-dione, 9-methoxy-11,13-dimethyl-, (7E,9S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



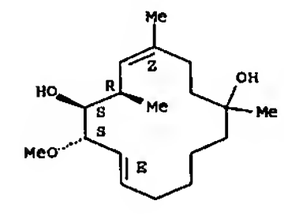
RN 760988-84-9 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4-dimethyl-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



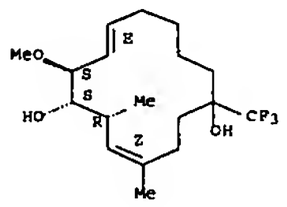
RN 760988-86-1 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4,7-trimethyl-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



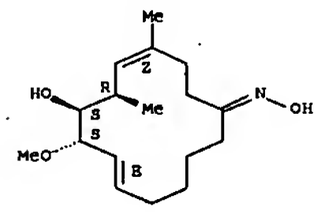
RN 760988-88-3 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4-dimethyl-7-(trifluoromethyl)-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 760988-89-4 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, oxime, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.

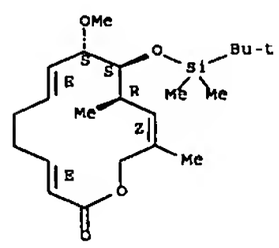


RN 760988-90-7 CAPLUS
CN 4,7,10,13-Tetraoxa-16-azaheneicosanoic acid, 21-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-17-oxo-, [(4Z,6R,7S,8S,9E)-7-hydroxy-8-methoxy-4,6-dimethyl-4,9-cyclotetradecadien-1-ylidene]hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.

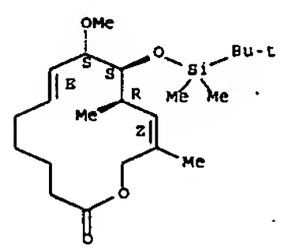
(3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



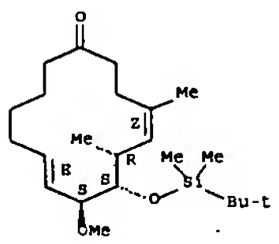
RN 663613-14-7 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

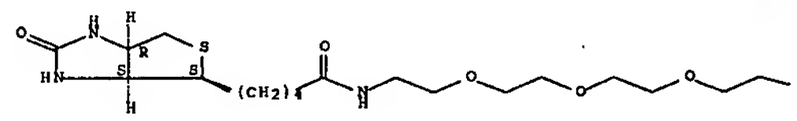


RN 663613-16-9 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

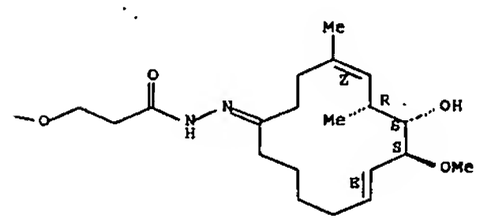
Absolute stereochemistry.
Double bond geometry as shown.



PAGE 1-A

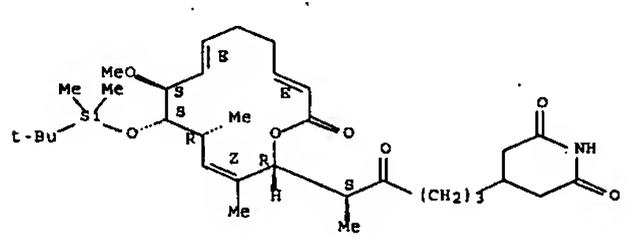


PAGE 1-B



IT 545339-21-7P 663613-13-6P 663613-14-7P
663613-16-9P 760988-66-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of migrastatin and analogs for pharmaceutical compns. to treat wounds, inhibit angiogenesis, cell proliferation, cell migration, tumor metastasis, and the structure-activity relationship)
RN 545339-21-7 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

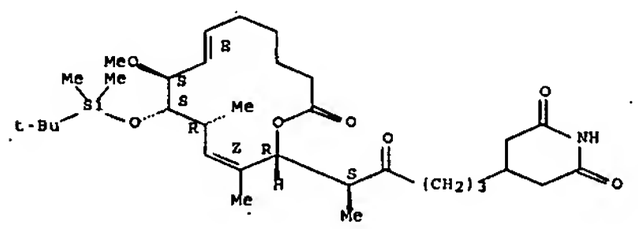
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-13-6 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-,

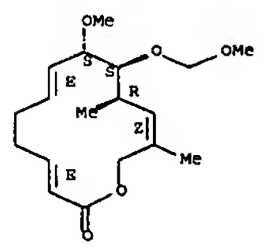
RN 760988-66-7 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 494834-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of migrastatin and analogs for pharmaceutical compns. to treat wounds, inhibit angiogenesis, cell proliferation, cell migration, tumor metastasis, and the structure-activity relationship)
RN 494834-82-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 9-methoxy-10-(methoxymethoxy)-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



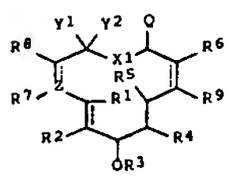
L13 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:857571 CAPLUS Full-text
DOCUMENT NUMBER: 141:349965
TITLE: Preparation of migrastatin analogs and their biological activity
INVENTOR(S): Huang, Xin-Yun; Danishefsky, Samuel J.; Gaul, Christoph; Njardarson, Jon T.

PATENT ASSIGNEE(S): Cornell Research Foundation, Inc., USA; Sloan-Kettering Institute for Cancer Research
SOURCE: PCT Int. Appl., 268 pp. CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087672	A1	20041014	WO 2004-US9380	20040326
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2520377	A1	20041014	CA 2004-2520377	20040326
EP 1608626	A1	20051228	EP 2004-758436	20040326
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
JP 2006523233	T	20061012	JP 2006-509369	20040326
US 2007037783	A1	20070215	US 2006-551152	20060925

PRIORITY APPLN. INFO.: US 2003-458827P P 20030328; US 2003-496165P P 20030819; WO 2004-US9380 W 20040326
OTHER SOURCE(S): CASREACT 141:349965; MARPAT 141:349965

GI



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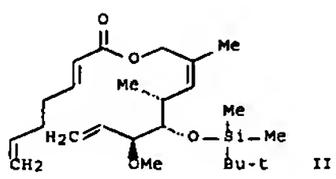

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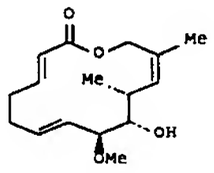


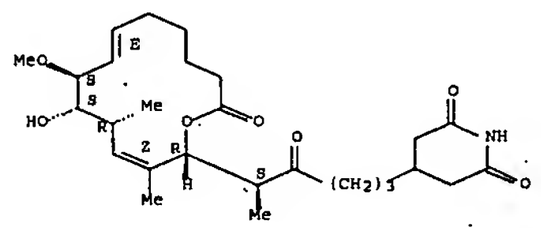
III

AB In one aspect, the present invention provides pharmaceutical compns. comprising a therapeutically effective amount of a compound of general formula I (R1, R2 = independently H, halide, cyano, NO2, etc.; R3 = H, alicyclic moiety, aryl, etc.; R4 = halide, OR10, NR10R11, R10, R11 = independently H, (hetero)aryl, alicyclic moiety, NR10R11 = heterocycle, heteroaryl; R5 = H, (hetero)aryl, (hetero)alicyclic, (hetero)aliphatic; R6 = H, halide, cyano, (hetero)aryl, amino, amido, etc.; R7, R8 = independently H, halide, cyano, amido, etc.; R7R8 = (hetero)aryl, (hetero)alicyclic; R9 = H, halide, cyano, sulfonyl, nitro, (hetero)aryl, etc.; R6R9 = (hetero)alicyclic, (hetero)aryl; Q = H, halide, cyano, sulfonyl, amido, etc.; X1 = O, S, amino, substituted carbon atom; Z = (CHR)n, n = 1-5; Y1, Y2 = independently H, (hetero) aliphatic, (hetero)aryl, etc.], whereby the composition is formulated for administration to a subject at a dosage between about 0.1 mg/kg to about 50 mg/kg of body weight In another aspect, the present invention provides a method for treating breast tumor metastasis in a subject comprising administering to a subject in need thereof a therapeutically effective amount of the inventive composition described directly above and a pharmaceutically acceptable carrier, adjuvant or vehicle. I are prepared via a ring-closing metathesis reaction. For example, tetraene II was prepared and treated with Grubbs' catalyst to give macrocyclic compound III after desilylation. III represents the core of migrastatin.

IT 663612-96-2P 663613-07-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological Study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of migrastatin and analogs for pharmaceutical compns. to treat wounds; inhibit angiogenesis, cell proliferation, cell migration, tumor metastasis; and the structure-activity relationship)

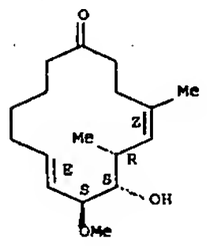
RN 663612-96-2 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 663613-07-8 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

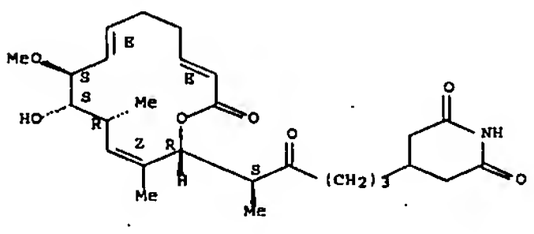
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT 314245-65-2P, Migrastatin 663612-97-3P
663612-00-1P 663613-01-2P 663613-10-3P
663613-11-4P 760988-87-8P 760988-88-9P
760988-94-5P 760988-96-1P 760988-98-3P
760988-89-4P 760988-90-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of migrastatin and analogs for pharmaceutical compns. to treat wounds; inhibit angiogenesis, cell proliferation, cell migration, tumor metastasis; and the structure-activity relationship)

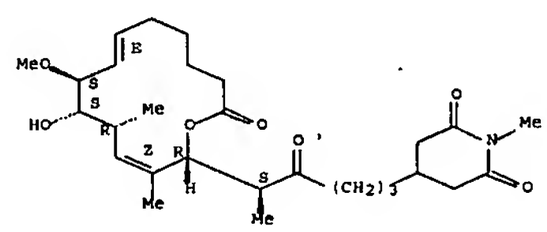
RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



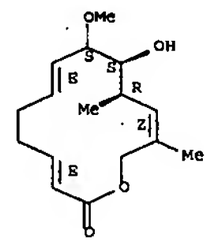
RN 663612-97-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]-1-methyl- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



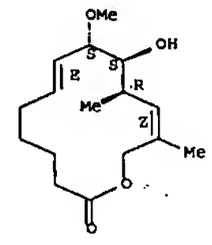
RN 663613-00-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-01-2 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

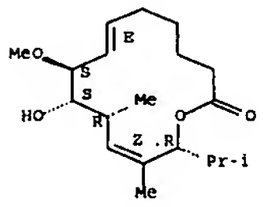
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-10-3 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-14-

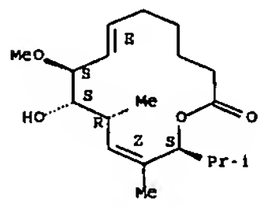
(1-methylethyl)-, (7E,9S,10S,11R,12Z,14R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



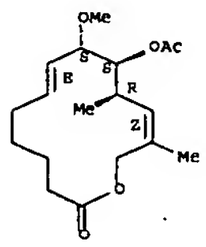
RN 663613-11-4 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-14-(1-methylethyl)-, (7E,9S,10S,11R,12Z,14S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



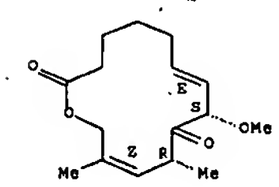
RN 760988-67-8 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-(acetyloxy)-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



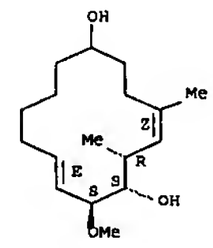
RN 760988-68-9 CAPLUS
CN Oxacyclotetradeca-7,12-diene-2,10-dione, 9-methoxy-11,13-dimethyl-, (7E,9S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



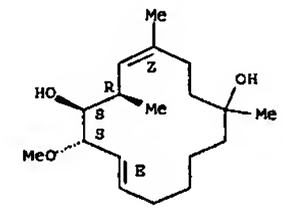
RN 760988-84-9 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4-dimethyl-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



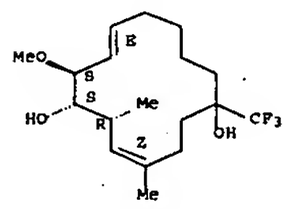
RN 760988-86-1 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4,7-trimethyl-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



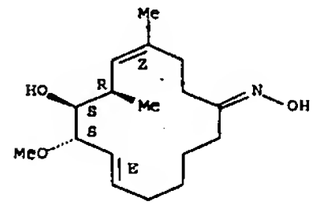
RN 760988-88-3 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4-dimethyl-7-(trifluoromethyl)-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 760988-89-4 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, oxime, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

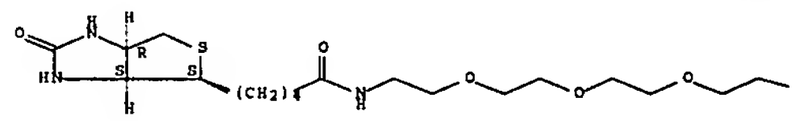
Absolute stereochemistry.
Double bond geometry as described by E or Z.



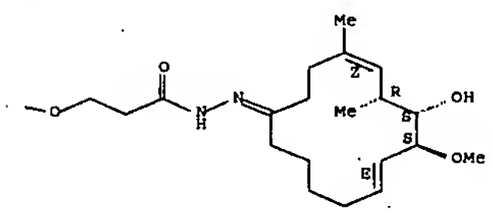
RN 760988-90-7 CAPLUS
CN 4,7,10,13-Tetraoxa-16-azaheneicosanoic acid, 21-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-17-oxo-, [(4Z,6R,7S,8S,9E)-7-hydroxy-8-methoxy-4,6-dimethyl-4,9-cyclotetradecadien-1-ylidene]hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.

PAGE 1-A



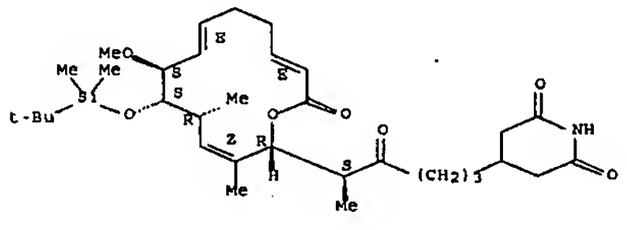
PAGE 1-B



IT 545339-21-7P 663613-13-6P 663613-14-7P
663613-16-9P 760988-66-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of migrastatin and analogs for pharmaceutical compns. to treat wounds; inhibit angiogenesis, cell proliferation, cell migration, tumor metastasis; and the structure-activity relationship)

RN 545339-21-7 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

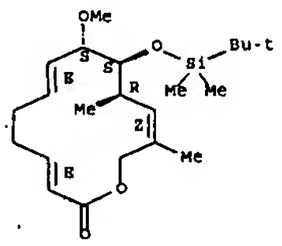
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-13-6 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-,

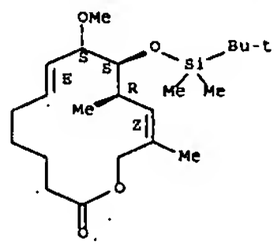
(3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



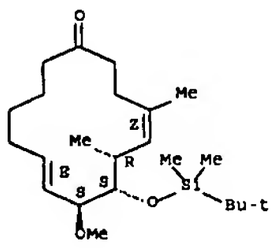
RN 663613-14-7 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



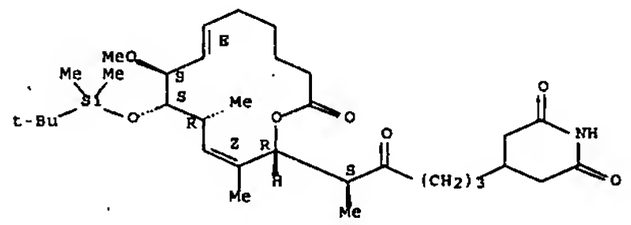
RN 663613-16-9 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



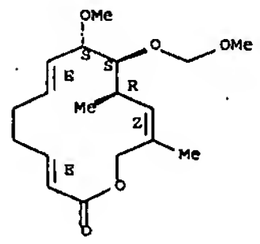
RN 760988-66-7 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 494834-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of migrastatin and analogs for pharmaceutical compns. to treat wounds; inhibit angiogenesis, cell proliferation, cell migration, tumor metastasis; and the structure-activity relationship)
RN 494834-82-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 9-methoxy-10-(methoxymethoxy)-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

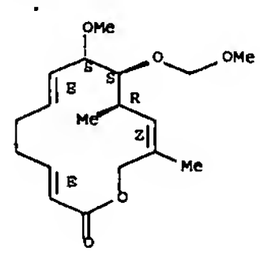
L13 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:607055 CAPLUS Full-text
DOCUMENT NUMBER: 141:295757
TITLE: The Migrastatin family: discovery of potent cell migration inhibitors by chemical synthesis

AUTHOR(S): Gaul, Christoph; Njardarson, Jon T.; Shan, Dandan; Dorn, David C.; Wu, Kai-Da; Tong, William P.; Huang, Xin-Yun; Moore, Malcolm A. S.; Danishefsky, Samuel J.
CORPORATE SOURCE: Laboratory for Bioorganic Chemistry, Sloan-Kettering Institute for Cancer Research, New York, NY, 10021, USA
SOURCE: Journal of the American Chemical Society (2004), 126(36), 11326-11337
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:295757.
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

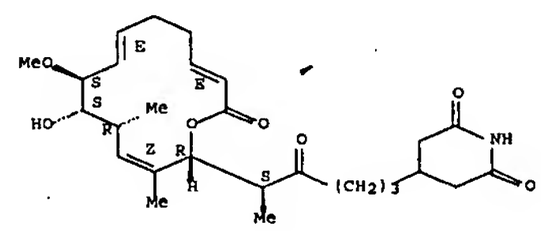
AB The first asym. total synthesis of (+)-migrastatin (I), a macrolide natural product with anti-metastatic properties, has been accomplished. Our concise and flexible approach utilized a Lewis acid-catalyzed diene aldehyde condensation (LACDAC) to install the three contiguous stereocenters and the trisubstituted (Z)-alkene of migrastatin. Construction of the two remaining stereocenters and incorporation of the glutarimide-containing side chain was achieved by an anti-selective aldol addition of propionyl oxazolidinone II to angelic aldehyde III (TBDMS = SiMe2CMe3), followed by a Horner-Wadsworth-Emmons (HWE) coupling of IV with 4-(2-oxoethyl)glutarimide. Finally, the assembly of the macrocycle was realized by a highly (E)-selective ring-closing metathesis. Utilizing the power of diverted total synthesis (DTS), a series of otherwise inaccessible analogs was prepared and evaluated for their potential as tumor cell migration inhibitors in several in vitro assays. These studies revealed a dramatic increase in activity when the natural motif was considerably simplified, presenting macrolactones V (X = O; dashed line = double bond) and V (X = O; dashed line = single bond) , as well as macrolactam V (X = NH; dashed line = single bond), macroketone V (X = CH2; dashed line = single bond), and CF3-alc. VI as promising anti-metastatic agents.
IT 494834-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(model compound; synthesis of migrastatin and related potent macrocyclic cell migration inhibitors)
RN 494834-82-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 9-methoxy-10-(methoxymethoxy)-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



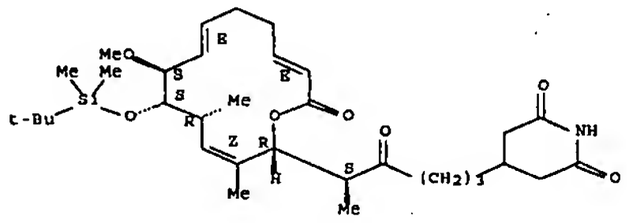
IT 314245-65-3P, (+)-Migrastatin
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and conjugate reduction of, with Stryker reagent; synthesis of migrastatin and related potent macrocyclic cell migration inhibitors)
RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



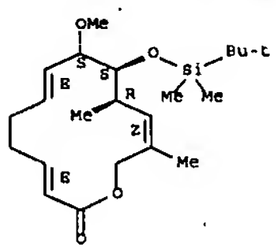
IT 545339-21-7P 663613-13-6P 663613-14-7P
663613-16-9P 760988-66-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desilylation of; synthesis of migrastatin and related potent macrocyclic cell migration inhibitors)
RN 545339-21-7 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



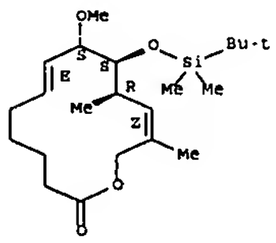
RN 663613-13-6 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 663613-14-7 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

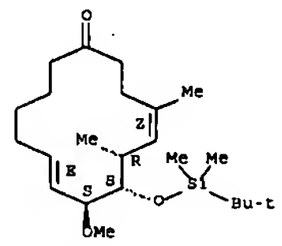
Absolute stereochemistry.
Double bond geometry as shown.



RN 663613-16-9 CAPLUS

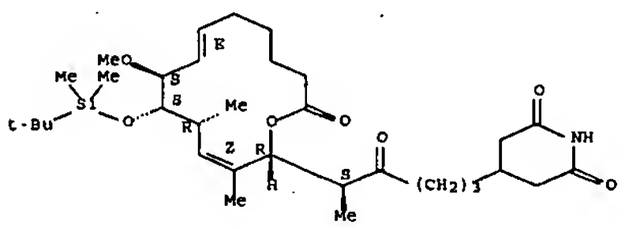
CN 4,9-Cyclotetradecadien-1-one, 7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



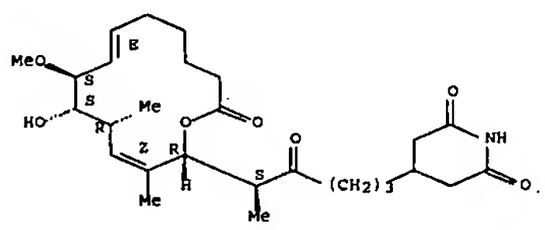
RN 760988-66-7 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



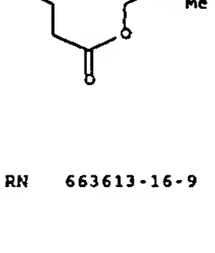
IT 663613-96-2P, 2,3-Dihydromigrastatin
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, N-methylation and cell migration inhibition by; synthesis of migrastatin and related potent macrocyclic cell migration inhibitors)
RN 663612-96-2 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



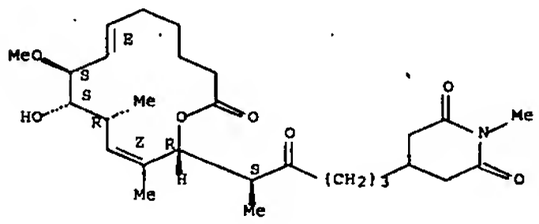
IT 663613-01-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, transformations and cell migration inhibition by; synthesis of migrastatin and related potent macrocyclic cell migration inhibitors)
RN 663613-01-2 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



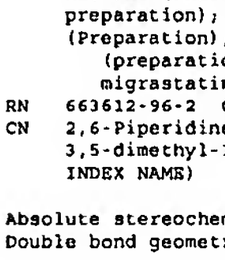
IT 663612-97-3P, N-Methyl-2,3-Dihydromigrastatin 663613-00-1P
663613-07-8P 663613-10-3P 663613-11-4P
760988-67-8P 760988-68-9P 760988-84-3P
760988-86-1P 760988-88-3P 760988-89-4P
760988-90-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of migrastatin and related potent macrocyclic cell migration inhibitors)
RN 663612-97-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]-1-methyl- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



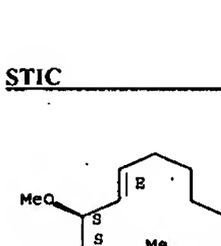
RN 663613-00-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-07-8 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

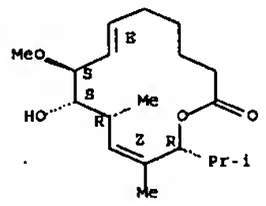
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-10-3 CAPLUS

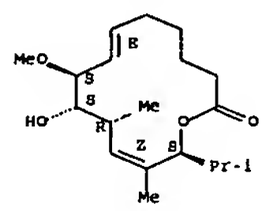
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-14-(1-methylethyl)-, (7E,9S,10S,11R,12Z,14R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



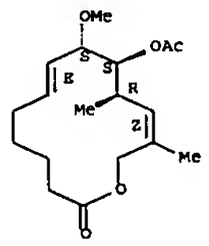
RN 663613-11-4 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-14-(1-methylethyl)-, (7E,9S,10S,11R,12Z,14S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



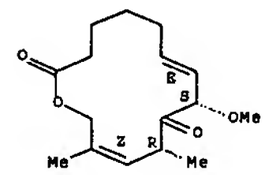
RN 760988-67-8 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-(acetyloxy)-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



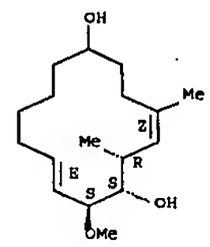
RN 760988-68-9 CAPLUS
CN Oxacyclotetradeca-7,12-diene-2,10-dione, 9-methoxy-11,13-dimethyl-, (7E,9S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



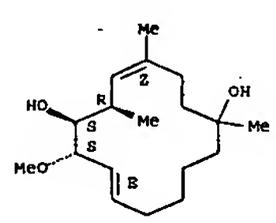
RN 760988-84-9 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4-dimethyl-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



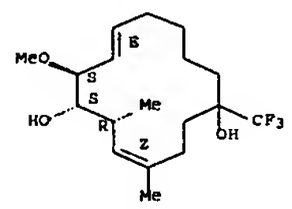
RN 760988-86-1 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4,7-trimethyl-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



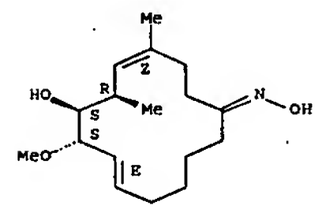
RN 760988-88-3 CAPLUS
CN 3,12-Cyclotetradecadiene-1,7-diol, 14-methoxy-2,4-dimethyl-7-(trifluoromethyl)-, (1S,2R,3Z,12E,14S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 760988-89-4 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, oxime, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

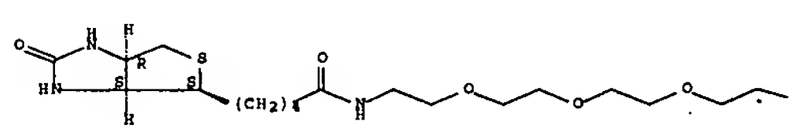
Absolute stereochemistry.
Double bond geometry as described by E or Z.



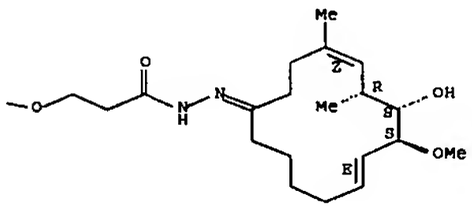
RN 760988-90-7 CAPLUS
CN 4,7,10,13-Tetraoxa-16-azaheneicosanoic acid, 21-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-17-oxo-, [(4Z,6R,7S,8S,9E)-7-hydroxy-8-methoxy-4,6-dimethyl-4,9-cyclotetradecadien-1-ylidene]hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.

PAGE 1-A



PAGE 1-B



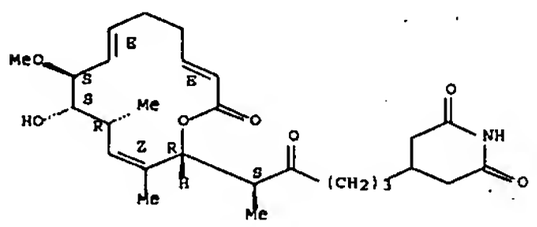
REFERENCE COUNT: 108 THERE ARE 108 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:8166 CAPLUS Full-text
DOCUMENT NUMBER: 140:199127
TITLE: Discovery of Potent Cell Migration Inhibitors through Total Synthesis: Lessons from Structure-Activity Studies of (+)-Migrastatin
AUTHOR(S): Njardarson, Jon T.; Gaul, Christoph; Shan, Dandan; Huang, Xin-Yun; Danishefsky, Samuel J.
CORPORATE SOURCE: Laboratory for Bioorganic Chemistry, Sloan-Kettering Institute for Cancer Research, New York, NY, 10021, USA
SOURCE: Journal of the American Chemical Society (2004), 126(4), 1038-1040
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:199127
AB Synthesis of highly active migrastatin-based tumor migration cell inhibitors was accomplished. Our flexible and concise total synthesis of migrastatin has allowed for the exploration of otherwise inaccessible migrastatin-derived structural motifs. This effort resulted in the discovery of analogs with tumor cell migration inhibitory activity 3 orders of magnitude higher than that of the natural product.
IT 314245-65-2

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(preparation of analogs of (+)-migrastatin from an advanced intermediate and
their activity as tumor cell migration inhibitors)

RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

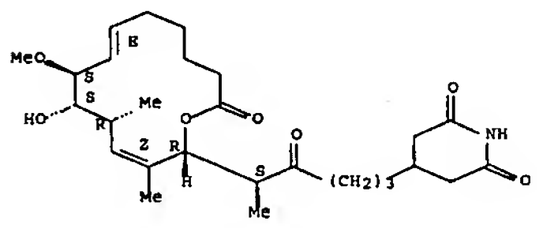
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT 663612-96-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of analogs of (+)-migrastatin from an advanced intermediate and
their activity as tumor cell migration inhibitors)

RN 663612-96-2 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

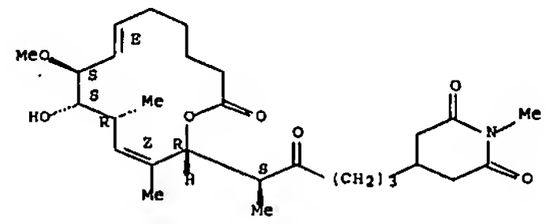


IT 663612-97-3P 663613-00-1P 663613-01-2P
663613-07-8P 663613-10-3P 663613-11-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

(Biological study); PREP (Preparation)
(preparation of analogs of (+)-migrastatin from an advanced intermediate and
their activity as tumor cell migration inhibitors)

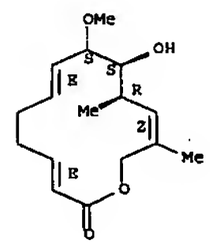
RN 663612-97-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]-1-methyl- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



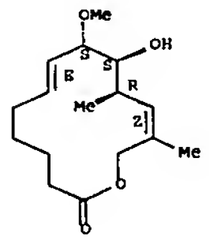
RN 663613-00-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



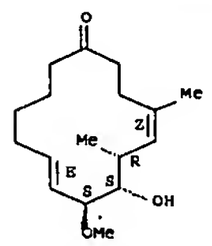
RN 663613-01-2 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



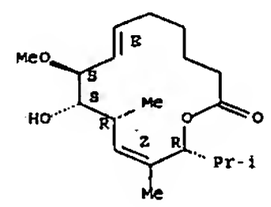
RN 663613-07-8 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



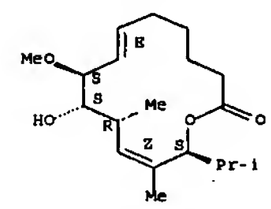
RN 663613-10-3 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-14-(1-methylethyl)-, (7E,9S,10S,11R,12Z,14R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 663613-11-4 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-hydroxy-9-methoxy-11,13-dimethyl-14-(1-methylethyl)-, (7E,9S,10S,11R,12Z,14S)- (CA INDEX NAME)

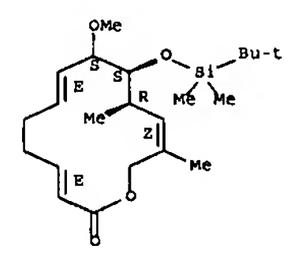
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT 663613-13-6P 663613-14-7P 663613-16-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of analogs of (+)-migrastatin from an advanced intermediate and
their activity as tumor cell migration inhibitors)

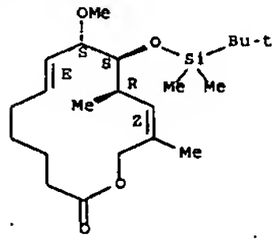
RN 663613-13-6 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



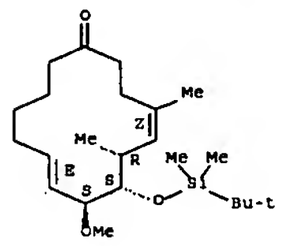
RN 663613-14-7 CAPLUS
CN Oxacyclotetradeca-7,12-dien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methoxy-11,13-dimethyl-, (7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 663613-16-9 CAPLUS
CN 4,9-Cyclotetradecadien-1-one, 7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

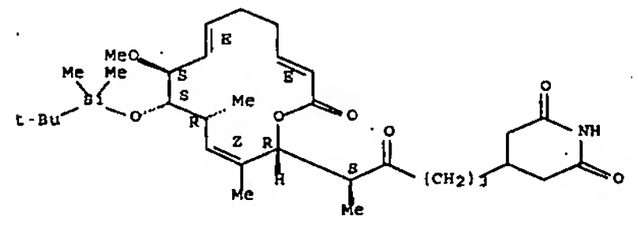
L13 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:323967 CAPLUS Full-text
DOCUMENT NUMBER: 139:52771
TITLE: The Total Synthesis of (+)-Migrastatin
AUTHOR(S): Gaul, Christoph; Njardarson, Jon T.; Danishefsky, Samuel J.
CORPORATE SOURCE: Laboratory for Bioorganic Chemistry, Sloan-Kettering Institute for Cancer Research, New York, NY, 10021, USA
SOURCE: Journal of the American Chemical Society (2003), 125(20), 6042-6043
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:52771

AB The first total synthesis of (+)-migrastatin, a macrolide natural product with interesting antimetastatic properties, has been accomplished. Our concise and flexible approach utilizes a Lewis acid-catalyzed diene aldehyde condensation of (E,Z)-MeOCH:CMeC(OSiMe3):CHMe with (S)-H2C:CHCH(OMe)CHO, to install the three contiguous stereocenters and the trisubstituted (Z)-alkene of

migrastatin. Construction of the two remaining stereocenters and incorporation of the glutarimide-containing side chain have been achieved via an anti-selective aldol reaction, followed by a Horner-Wadsworth-Emmons olefination. Finally, the assembly of the macrocycle has been realized by a highly (E)-selective ring-closing metathesis.

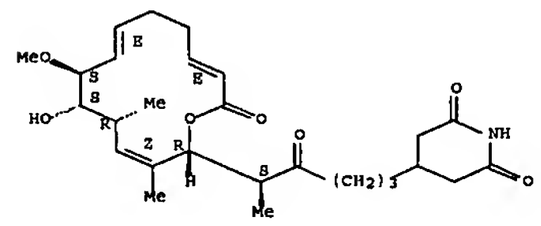
IT 545339-21-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of (+)-migrastatin via diene-aldehyde condensation, anti-selective aldol, Horner-Wadsworth-Emmons olefination, and ring-closing metathesis)
RN 545339-21-7 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



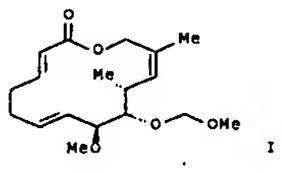
IT 314245-65-3P, (+)-Migrastatin
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of (+)-migrastatin via diene-aldehyde condensation, anti-selective aldol, Horner-Wadsworth-Emmons olefination, and ring-closing metathesis)
RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:862418 CAPLUS Full-text
DOCUMENT NUMBER: 138:153349
TITLE: Synthesis of the macrolide core of migrastatin
AUTHOR(S): Gaul, Christoph; Danishefsky, Samuel J.
CORPORATE SOURCE: Laboratory for Bioorganic Chemistry, Sloan-Kettering Institute for Cancer Research, New York, NY, 10021, USA
SOURCE: Tetrahedron Letters (2002), 43(50), 9039-9042
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:153349
GI

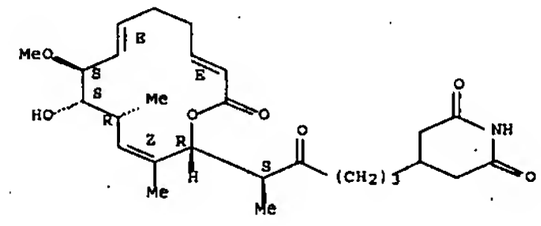


I

AB A concise and efficient synthesis of the macrolactone core I of migrastatin, a new natural product with potent anticancer properties, has been achieved. The key features of our synthetic strategy encompass a Lewis acid catalyzed diene aldehyde condensation (LACDAC) to install the three contiguous stereocenters and the trisubstituted (Z)-double bond of migrastatin, and a (E)-selective ring-closing metathesis (RCM) to construct the macrocycle.

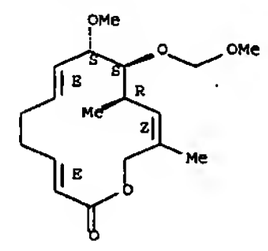
IT 314245-65-3P, Migrastatin
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of the macrolactone core of migrastatin utilizing lewis acid catalyzed diene aldehyde condensation and ring-closing metathesis)
RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT 494834-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of the macrolactone core of migrastatin utilizing lewis acid catalyzed diene aldehyde condensation and ring-closing metathesis)
RN 494834-82-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 9-methoxy-10-(methoxymethoxy)-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:658739 CAPLUS Full-text
DOCUMENT NUMBER: 137:184573
TITLE: Fermentation and purification of migrastatin and analog
INVENTOR(S): Khosla, Chaitan; Licari, Peter; Carney, John
PATENT ASSIGNEE(S): Kosan Biosciences, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 7 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002119937	A1	20020829	US 2001-932167	20010817

US 6750047 B2 20040615
US 2004209336 A1 20041021 US 2004-838895 20040503
PRIORITY APPLN. INFO.: US 2000-226595P P 20000821
US 2001-932167 A3 20010817

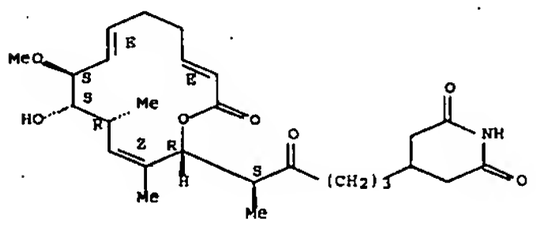
AB Migrastatin and a migrastatin analog can be produced by fermentation of Streptomyces platensis NRRL 18993 and used in pharmaceutical formulations to treat cancer and/or inhibit metastasis of cancer cells.

IT 314245-65-3P, Migrastatin
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(fermentation and purification of migrastatin and analog)

RN 314245-65-3 CAPLUS

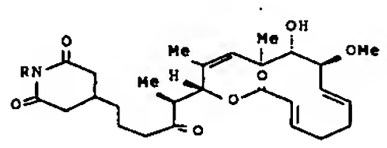
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:340580 CAPLUS Full-text
DOCUMENT NUMBER: 137:154778
TITLE: Absolute configuration of migrastatin, a novel 14-membered ring macrolide. Comments.
AUTHOR(S): Nakamura, Hiraku
CORPORATE SOURCE: Japan
SOURCE: Journal of Antibiotics (2002), 55(4), 442-444
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:154778
GI



I

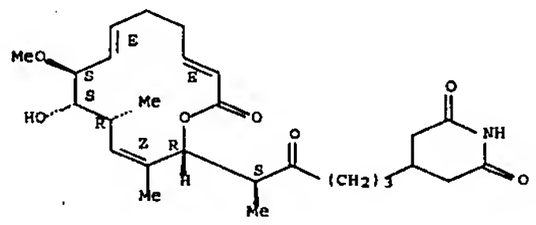
AB The X-ray crystallog. anal. of N-p-bromophenacylmigrastatin I (R = CH2CO-p-C6H4-Br) led the establishment of absolute configuration of migrastatin I (R = H), a novel 14-membered ring macrolide, isolated from a culture broth of Streptomyces sp. MK929-43F1.

IT 314245-65-3
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(determination of absolute configuration of migrastatin via X-ray crystallog. anal.
of N-p-bromophenacylmigrastatin)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:203151 CAPLUS Full-text
DOCUMENT NUMBER: 136:339536
TITLE: Migrastatin and a new compound, isomigrastatin, from Streptomyces platensis
AUTHOR(S): Woo, Elaine J.; Starks, Courtney M.; Carney, John R.; Arslanian, Robert; Cadapan, Lawrence; Zavala, Stefan; Licari, Peter
CORPORATE SOURCE: Kosan Biosciences, Inc., Hayward, CA, 94545, USA
SOURCE: Journal of Antibiotics (2002), 55(2), 141-146
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:339536

AB Streptomyces platensis (strain NRRL 18993), a producer of dorrigocins, was shown to produce migrastatin, a cyclic congener of dorrigocin A previously reported from a different organism. Addnl. a new compound isomeric to migrastatin, isomigrastatin, was also isolated and its structure was determined to be a cyclic form of dorrigocin B. Both compds. were fully

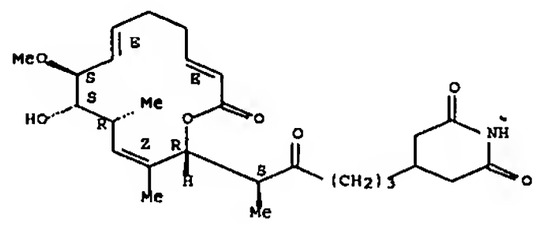
characterized from MS and NMR data. Product titers of both were improved by the addition of XAD-16 resin to the fermentation medium.

IT 314245-65-3P, Migrastatin
RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(migrastatin and its isomer isomigrastatin from Streptomyces platensis fermentation)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:11968 CAPLUS Full-text
DOCUMENT NUMBER: 136:226436
TITLE: Migrastatin, a novel 14-membered ring macrolide, inhibits anchorage-independent growth of human small cell lung carcinoma Ms-1 cells
AUTHOR(S): Takemoto, Yasushi; Nakae, Koichi; Kawatani, Makoto; Takahashi, Yoshikazu; Naganawa, Hiroshi; Imoto, Masaya
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Science and Technology, Keio University, Yokohama, 223-8522, Japan
SOURCE: Journal of Antibiotics (2001), 54(12), 1104-1107
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effects of teleocidin-free migrastatin on tumor cell migration and on the growth of several types of tumor cells were reported. The original migrastatin contained about 0.1% teleocidin-related compds. Migrastatin inhibited migration of EC17 cells with an IC50 value of approx. 10μg/mL, but it inhibited cell proliferation of EC17 cells with an IC50 value of 82μg/mL, and it failed to induce cell death in EC17 cells up to 100 μg/mL. These results showed that the inhibited migration of EC17 cells by migrastatin should not be due to the inhibition of cell proliferation or induction cell death by the drug. Migrastatin did not considerably reduced the growth rate up to 30μg/mL, and 100μg/mL of migrastatin induced cell death as evaluated by

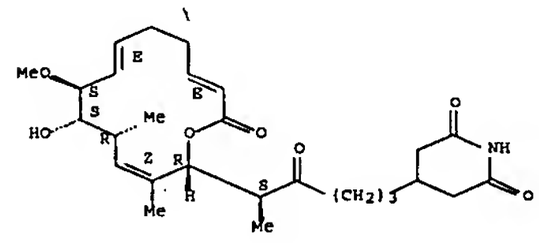
trypan blue dye exclusion assay. It reduced the anchorage-independent growth ability of Ms-1 cells. The growth rate of Ms-1 cells under anchorage-independent condition was lower than that under anchorage-dependent condition.

IT 314245-65-3, Migrastatin
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(migrastatin inhibits anchorage-independent growth of human small cell lung carcinoma Ms-1 cells)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

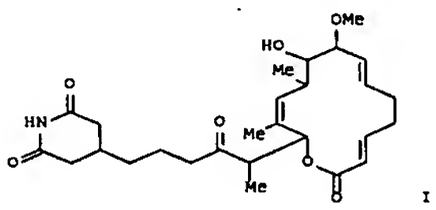


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:472958 CAPLUS Full-text
DOCUMENT NUMBER: 135:45279
TITLE: Migrastatin, process for producing the same and medicinal compositions
INVENTOR(S): Takeuchi, Tomio; Sawa, Tsutomu; Hamada, Masa; Naganawa, Hiroshi; Takahashi, Yoshigazu; Imoto, Masaya; Nakae, Kouichi
PATENT ASSIGNEE(S): Zaidan Hojin Biseibutsu Kagaku Kenkyu Kai, Japan
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046451	A1	20010628	WO 2000-JP9147	20001222
W: AU, CA, CN, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
PRIORITY APPLN. INFO.:			JP 1999-364316	A 19991222

GI



I

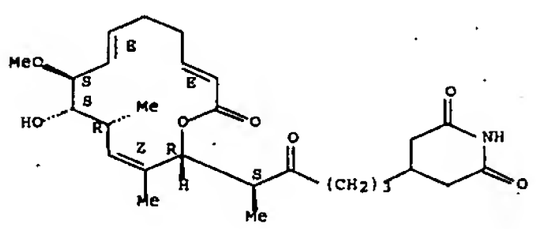
AB Migrastatin (I) is manufactured by culturing Streptomyces sp. MK929-43F1. Migrastatin has an anticancer activity against various human cancers or tumor cells, a cell motility inhibitory activity, and an angiogenesis inhibitory activity on vascular endothelial cells. Shake-culture of Streptomyces and purification of I by filtration, solvent extraction, and chromatog. was shown.

IT 314245-65-3P, Migrastatin
RL: BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Migrastatin, process for producing the same and medicinal compns.)

RN 314245-65-3 CAPLUS

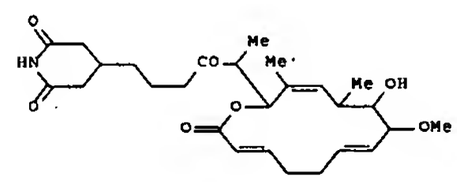
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:780072 CAPLUS Full-text
DOCUMENT NUMBER: 134:71413
TITLE: Migrastatin, a novel 14-membered lactone from Streptomyces sp. MK929-43F1
AUTHOR(S): Nakae, Koichi; Yoshimoto, Yuya; Ueda, Minoru; Sawa, Tsutomu; Takahashi, Yoshikazu; Naganawa, Hiroshi; Takeuchi, Tomio; Imoto, Masaya
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Science and Technology, Keio University, Yokohama, 223, Japan
SOURCE: Journal of Antibiotics (2000), 53(10), 1228-1230
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

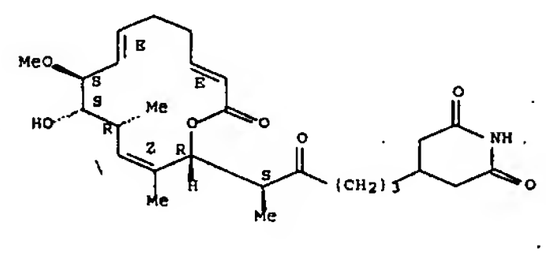
AB The mol. structure and olefinic bond geometry of migrastatin (I), a novel 14-membered lactone from Streptomyces sp. MK929-43F1, was determined by spectral means.

IT 314245-65-3, Migrastatin
RL: PRP (Properties)
(mol. structure of migrastatin, a novel 14-membered lactone previously isolated from Streptomyces sp. MK929-43F1)

RN 314245-65-3 CAPLUS

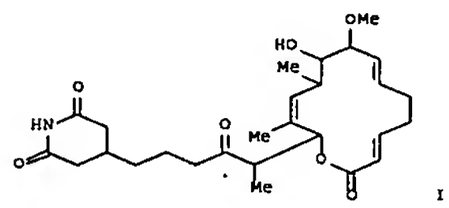
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:780057 CAPLUS Full-text
DOCUMENT NUMBER: 134:68523
TITLE: Migrastatin, a new inhibitor of tumor cell migration from Streptomyces sp. MK929-43F1. Taxonomy, fermentation, isolation and biological activities
AUTHOR(S): Nakae, Koichi; Yoshimoto, Yuya; Sawa, Tsutomu; Homma, Yoshiko; Hamada, Masa; Takeuchi, Tomio; Imoto, Masaya
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Science and Technology, Keio University, Yokohama, 223-8522, Japan
SOURCE: Journal of Antibiotics (2000), 53(10), 1130-1136
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A new compound, migrastatin (I), was isolated from a cultured broth of Streptomyces sp. MK929-43F1, as an inhibitor of tumor cell migration. It was purified by column chromatogs. on silica gel and Sephadex LH-20 and HPLC. I has the mol. formula of C27H39NO7 consisting of 14-membered macrolide and glutarimide moiety. It inhibited spontaneous migration of human esophageal cancer EC17 cells. Migration inhibitory activity of I was not dependent on cytotoxicity or inhibition of protein synthesis.

IT 314245-65-3P, Migrastatin
RL: BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(migrastatin is a new inhibitor of tumor cell migration from Streptomyces MK929-43F1)

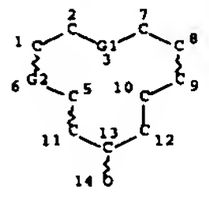
RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

Sample of results from broad structure search:

=> d que l14
L1 STR



VAR G1=O/S/N/C
REP G2=(1-5) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

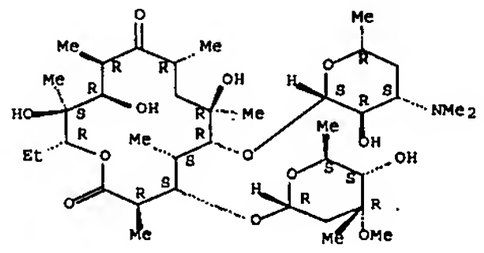
STEREO ATTRIBUTES: NONE
L3 58774 SEA FILE=REGISTRY ABB=ON PLU=ON C12/ESS OR C13/ESS OR C14/ESS OR C15/ESS OR C16/ESS
L4 53366 SEA FILE=REGISTRY ABB=ON PLU=ON OC11/ESS OR OC12/ESS OR OC13/ESS OR OC14/ESS OR OC15/ESS
L5 417 SEA FILE=REGISTRY ABB=ON PLU=ON SC11/ESS OR SC12/ESS OR SC13/ESS OR SC14/ESS OR SC15/ESS
L6 3857 SEA FILE=REGISTRY ABB=ON PLU=ON NC11/ESS OR NC12/ESS OR NC13/ESS OR NC14/ESS OR NC15/ESS
L7 116341 SEA FILE=REGISTRY ABB=ON PLU=ON (L3 OR L4 OR L5 OR L6)
L9 25195 SEA FILE=REGISTRY SUB=L7 SSS FUL L1
L14 25691 SEA FILE=CAPLUS ABB=ON PLU=ON L9

=> d l14 ibib abs hitstr 1000-1002 20000-20002 25690-25691

L14 ANSWER 1000 OF 25691 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:192267 CAPLUS Full-text
DOCUMENT NUMBER: 147:137631
TITLE: Detection of disinfectant-resistant gene qacA/B of methicillin resistant Staphylococcus aureus
AUTHOR(S): Mo, Fei; Wan, Shan; Fei, Ying; Tan, Gui-lin
CORPORATE SOURCE: Dep. of Clinical Laboratory, Guiyang Medical College, Guiyang, Guizhou, 550004, Peop. Rep. China
SOURCE: Guiyang Yixueyuan Xuebao (2006), 31(6), 567-568
CODEN: GYXUE7; ISSN: 1000-2707
PUBLISHER: Guiyang Yixueyuan Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB This paper detected the disinfectant-resistant gene qacA/B of methicillin resistant Staphylococcus aureus (MRSA). PCR and gel electrophoresis were used to detect the qacA/B gene and mecA gene in MRSA. Drug susceptibility test in

20 strains of MRSA was processed. The results showed that among 20 strains of MRSA, 19 (95%) strains were mecA pos. and 8 (40%) strains were qacA/B pos. MRSA showed whole resistance to oxazacillin, penicillin, cefoxitin, erythromycin and clindamycin, and the resistance rate of MRSA to sulphamethoxazole, gentamicin, tetracycline, levofloxacin and rifampicin was 90%, 75%, 75%, 70%, and 55% resp. MRSA was sensitive to teicoplanin, vancomycin, quinupristin-dalfopristin, fusidic acid, and nitrofurantoin.
IT 114-07-8, Erythromycin
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(detection of disinfectant-resistant gene qacA/B of methicillin resistant Staphylococcus aureus)
RN 114-07-8 CAPLUS
CN Erythromycin (CA INDEX NAME)

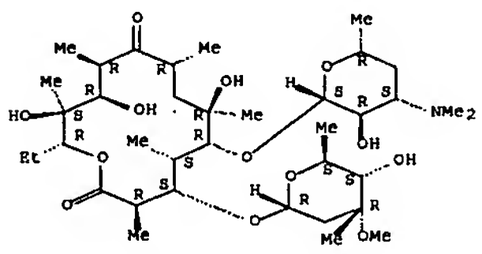
Absolute stereochemistry. Rotation (-).



L14 ANSWER 1001 OF 25691 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:191554 CAPLUS Full-text
DOCUMENT NUMBER: 146:330762
TITLE: Determination of Phospholipidosis Potential Based on Gene Expression Analysis in HepG2 Cells
AUTHOR(S): Atienzar, Franck; Gerets, Helga; Dufrane, Simon; Tilmant, Karen; Cornet, Miranda; Dhalluin, Stephane; Ruty, Bernard; Rose, Geoffrey; Canning, Michael
CORPORATE SOURCE: Non-Clinical Development, Chemin du Foriest, UCB Pharma SA, Braine-l'Alleud, 1420, Belg.
SOURCE: Toxicological Sciences (2007), 96(1), 101-114
CODEN: TOSCF2; ISSN: 1096-6080
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phospholipidosis (PLD) is characterized by an intracellular accumulation of phospholipids in lysosomes and the concurrent development of concentric lamellar bodies. Recently, H. Sawada et al. (2005, Toxicol. Sci. 83, 282-292) identified 17 genes as potential biomarkers of PLD in HepG2 cells. The present study was undertaken to determine if this set of genes measured by quant. PCR could be validated in the same cell line. The objective was also to investigate the dose-response relationship to further validate the assay and to select the concns. to use for screening activities. In a first experiment (one concentration tested), out of the 17 genes, the best gene biomarkers of PLD (i.e., 11 genes) were selected for practical screening reasons. Based on these genes, 91.6% (i.e., 11 of 12) of the compds. known to induce PLD were identified as pos. and all the neg. compds. (i.e., five of

five) were also confirmed. When the data obtained in the first experiment were compared to the data by Sawada et al., (2005) the coefficient of correlation calculated was slightly higher than 75%. In the second experiment (26 compds. [all 17 compds. from the first experiment plus 9 other compds.] tested at a min. of three concns.), 93.3% (14/15) of the compds. known to induce PLD were identified as such and all the neg. controls (six compds.) were also confirmed. Three compds. likely to induce PLD were identified as pos. in our assay. Finally, two compds. for which no data are available were also tested. When both expts. 1 and 2 were compared, the coefficient of correlation for 16 compds. tested at the same concns. reached 87.7%. In conclusion, the present study further confirms the utility of gene expression in HepG2 cells to identify a potential to induce PLD. Finally, based on the data presented, researchers are encouraged to use a range of min. three concns. (e.g., 12.5, 25, and 50μM) to screen for PLD in the human HepG2 cell line.
IT 114-07-8, Erythromycin
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(determination of drug-induced phospholipidosis based on gene expression anal.
in HepG2 cells)
RN 114-07-8 CAPLUS
CN Erythromycin (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

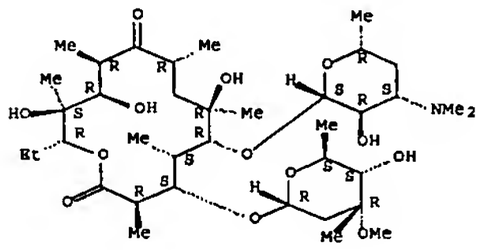
L14 ANSWER 1002 OF 25691 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:191160 CAPLUS Full-text
DOCUMENT NUMBER: 147:413517
TITLE: Determination of two antibacterial binary mixtures by chemometrics-assisted spectrophotometry
AUTHOR(S): Mohamed, Abd El-Maaboud I.; Abdelmageed, Osama H.; Refaat, Ibrahim H.
CORPORATE SOURCE: Faculty of Pharmacy, Department of Pharmaceutical Analytical Chemistry, Assiut University, Assiut, Egypt
SOURCE: Journal of AOAC International (2007), 90(1), 128-141
CODEN: JAINEE; ISSN: 1060-3271
PUBLISHER: AOAC International
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Simple chemometrics-assisted spectrophotometric methods are described for determination of 2 antibacterial binary mixts. The mixts. are composed of

norfloxacin in combination with tinidazole and erythromycin (as ethylsuccinate ester or stearate salt) in combination with trimethoprim. The normal UV absorption spectra of each pair of drugs in the studied mixts., in the range of 200-400 nm, showed a considerable degree of spectral overlapping: 77.5% for the norfloxacin-tinidazole mixture and 84.3% for the erythromycin-trimethoprim mixture Resolution of the norfloxacin-tinidazole mixture and trimethoprim in the presence of erythromycin was accomplished successfully by using zero-crossing first derivative (1D), classical least-squares (CLS) regression anal., and principal component regression (PCR) anal. methods. In addition, an alternative simple and accurate colorimetric method was developed for the determination of erythromycin in the presence of trimethoprim using 2,4-dinitrophenylhydrazine. All variables affecting the development of the colored chromogen were studied and optimized, and the product was measured at 526-529 and 538-542 nm for erythromycin stearate and erythromycin ethylsuccinate, resp. For zero-crossing, first derivative technique Beer's law was obeyed in the general concentration range of 2-50 μg/mL for norfloxacin, tinidazole, and trimethoprim with good correlation coeffs. (0.9994-0.9996). Overall limits of detection (LOD) and quantification (LOQ) ranged from 0.59 to 2.81 and 1.96 to 9.33 μg/mL, resp. The obtained results from CLS and PCR were compared with those obtained from a 1D spectrophotometric method. With the exception of erythromycin, overall recoveries in the average range of 97.33-103.0% were obtained with a considerable degree of accuracy when the suggested methods were applied to anal. of synthetic binary mixts., some com. dosage forms such as tablets and oral suspension without interference from the commonly encountered excipients and additives. For the colorimetric method, Beer's law was obeyed in the general concentration range of 7.21-28.84 μg/mL erythromycin with good correlation coeffs. (0.9980-0.9996). Overall LOD and LOQ ranged from 0.73 to 1.65 and 2.43-5.49 μg/mL, resp. Erythromycin derivs. were determined in the com. dosage form, without interference from trimethoprim-encountered excipients and additives. The obtained results, with both chemometric and colorimetric methods, have been compared with those obtained from reported methods, and proper F- and t-values were observed, indicating no significant difference between the results of the suggested methods and reported method(s). The good percentage recoveries and proper statistical data obtained proved the efficiency of the proposed procedures for the determination of the studied drugs in their binary mixts. as well as in the com. dosage forms with quite satisfactory precision.
IT 643-22-1, Erythromycin stearate 1264-62-6, Erythromycin ethylsuccinate 992375-97-8, Primomycin 950905-61-9, Erythroprim
RL: ANT (Analyte); PRP (Properties); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(two antibacterial binary mixts. determination by chemometrics-assisted spectrophotometry)
RN 643-22-1 CAPLUS
CN Erythromycin, octadecanoate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 114-07-8
CMF C37 H67 N O13

Absolute stereochemistry. Rotation (-).



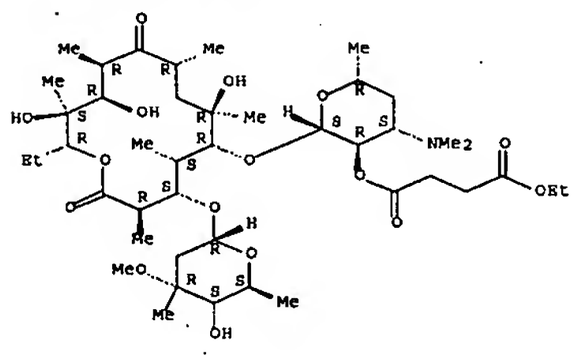
CM 2

CRN 57-11-4
CMF C18 H36 O2

$HO_2C-(CH_2)_{16}-Me$

RN 1264-62-6 CAPLUS
CN Erythromycin, 2'-(ethyl butanedioate) (CA INDEX NAME)

Absolute stereochemistry.

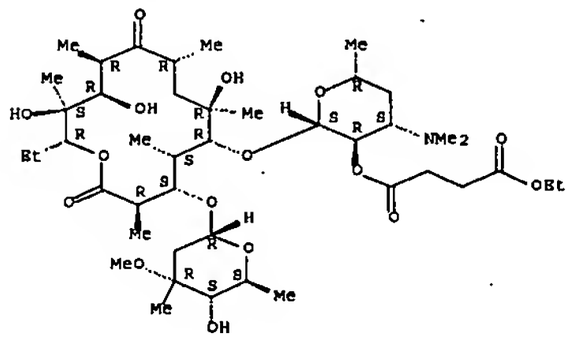


RN 932375-97-8 CAPLUS
CN Erythromycin, 2'-(4-ethyl butanedioate), mixt. with 5-[(3,4,5-trimethoxyphenyl)methyl]-2,4-pyrimidinediamine (CA INDEX NAME)

CM 1

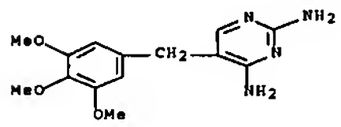
CRN 1264-62-6
CMF C43 H75 N O16

Absolute stereochemistry.



CM 2

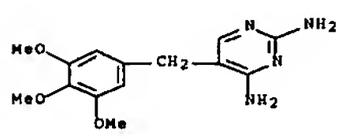
CRN 738-70-5
CMF C14 H18 N4 O3



RN 950905-61-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 738-70-5
CMF C14 H18 N4 O3



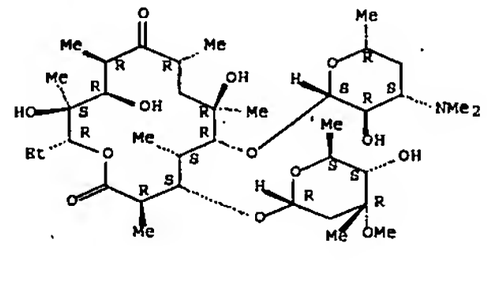
CM 2

CRN 643-22-1
CMF C37 H67 N O13 . C18 H36 O2

CM 3

CRN 114-07-8
CMF C37 H67 N O13

Absolute stereochemistry. Rotation (-).



CM 4

CRN 57-11-4
CMF C18 H36 O2

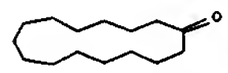
$HO_2C-(CH_2)_{16}-Me$

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

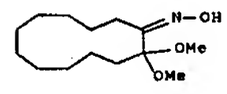
L14 ANSWER 20000 OF 25691 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:405860 CAPLUS Full-text
DOCUMENT NUMBER: 97:5860
TITLE: Cyclic ketones
PATENT ASSIGNEE(S): Daicel Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAP
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57024322	A	19820208	JP 1980-98258	19800718
JP 61011937	B	19860405		
US 4335261	A	19820615	US 1981-274682	19810617
PRIORITY APPLN. INFO.:			JP 1980-98258 A	19800718
OTHER SOURCE(S):	MARPAT 97:5860			

GI For diagram(s), see printed CA Issue.
AB I (n = 14-16), useful as perfumes, were prepared Thus, Dieckmann reaction of 220 g EtO2C(CH2)13CH2CO2Et followed by hydrolysis and decarboxylation gave 67.8 g I (n = 14).
IT 502-72-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 502-72-7 CAPLUS
CN Cyclopentadecanone (CA INDEX NAME)

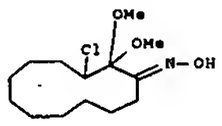


L14 ANSWER 20001 OF 25691 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:405832 CAPLUS Full-text
DOCUMENT NUMBER: 97:5832
TITLE: Reactions of 2,2-dialkoxy ketone oximes with chlorine and bromine. Halogenation vs. Beckmann fragmentation
AUTHOR(S): Oxenrider, Bryce C.; Rogic, Milorad M.
CORPORATE SOURCE: Corp. Res. Dev. Lab., Allied Corp., Morristown, NJ, 07960, USA
SOURCE: Journal of Organic Chemistry (1982), 47(13), 2629-33
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:5832
AB Reactions of 2,2-dialkoxycycloalkanone oximes with Cl or Br can be directed either to give 3-chloro- or 3-bromo-2,2-dialkoxycycloalkanone oximes or to undergo Beckmann fragmentation to give ω- (alkoxycarbonyl)alkanehydroximoyl halides. The resulting hydroximoyl halides can be converted either to the corresponding nitrile oxides, furoxan derivs., or they could be rearranged through the intermediacy of nitrile oxides into corresponding isocyanates. Catalyzed Beckmann fragmentation of 3-chloro-2,2-dimethoxycyclohexanone oxime provided Me 2-chloro-5-cyanovalerate, a useful lysine precursor.
IT 68226-33-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)
RN 68226-33-5 CAPLUS
CN Cyclododecanone, 2,2-dimethoxy-, oxime (9CI) (CA INDEX NAME)



IT 81617-28-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 81617-28-9 CAPLUS

CN Cyclododecanone, 3-chloro-2,2-dimethoxy-, oxime (9CI) (CA INDEX NAME)

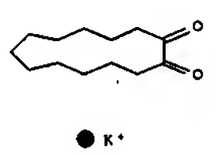


L14 ANSWER 20002 OF 25691 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:405560 CAPLUS Full-text
DOCUMENT NUMBER: 97:5560
TITLE: Aliphatic semidiones. 42. The cis-trans equilibriums in aliphatic semidiones
AUTHOR(S): Russell, Glen A.; Osuch, C. E.
CORPORATE SOURCE: Dep. Chem., Iowa State Univ., Ames, IA, 50011, USA
SOURCE: Journal of the American Chemical Society (1982), 104(12), 3353-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

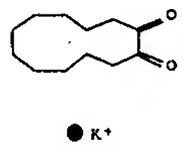
AB Ion pairing and cis-trans equilibrium of the dimethylsemidiones in Me2SO in the presence of K+ has been analyzed in terms of four equilibrium consts., which at 25° are as follows: trans free ion/cis free ion = 125 [ΔH°(trans-cis) = -2.5 kcal/mol]; trans ion pair/cis ion pair = 2 [ΔH°(trans-cis) = -1.4 kcal/mol]; ion pairing for the cis semidione = 250 M-1 (ΔH° = -1.1 kcal/mol); ion pairing for the trans semidione = 4 M-1 (ΔH° = 0). In cyclic C11 - C15 semidiones the cis and trans isomers can be detected. The cis isomers are favored by high [K+] whereas in the presence of K+-[2.2.2]-cryptand the trans isomers are preferred. The cyclic trans 1,2-semidiones exist in an asym. conformation with 4 magnetically nonequiv. α-H atoms, which become time averaged to two pairs of H atoms at higher temps. (>25° for C15 and >170° for C11). Internal rotation in the trans 1,2-cyclic semidiones is quite slow but can be detected for the trans-cyclopentadecane-1,2-semidione at 130°.

IT 70136-08-2 81572-63-6 81572-64-7
81583-51-9
RL: PRP (Properties)
(isomerism and ESR of)

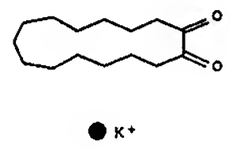
RN 70136-08-2 CAPLUS
CN 1,2-Cyclotridecanedione, radical ion(1-), potassium (9CI) (CA INDEX NAME)



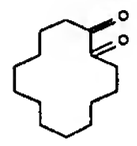
RN 81572-63-6 CAPLUS
CN 1,2-Cyclododecanedione, radical ion(1-), potassium (9CI) (CA INDEX NAME)



RN 81572-64-7 CAPLUS
CN 1,2-Cyclopentadecanedione, radical ion(1-), potassium (9CI) (CA INDEX NAME)



RN 81583-51-9 CAPLUS
CN 1,2-Cyclotetradecanedione, radical ion(1-), potassium (9CI) (CA INDEX NAME)



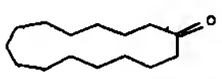
L14 ANSWER 25690 OF 25691 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1926:17678 CAPLUS Full-text
DOCUMENT NUMBER: 20:17678
ORIGINAL REFERENCE NO.: 20:2151b-g
TITLE: Carbon rings. VI. The relative ease of formation, the relative stability and the spatial structure of the saturated carbon rings
AUTHOR(S): Ruzicka, L.; Brugger, W.; Pfeiffer, M.; Schinz, H.; Stoll, M.
SOURCE: Helvetica Chimica Acta (1926), 9, 499-520
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

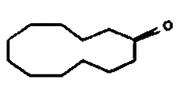
AB C rings with 5 or more members in the ring are characterized, as compared with the 3- and 4-membered rings, by a special stability towards the splitting of the ring. Only those C rings can be stable in which the valences of the ring members assume the same position as those of the aliphatic compds., i. e., they are equally or nearly equally distributed in space. It is possible to give space formulas only for the stable C rings which correspond to the last requirement. The ring members of the 6- and higher ring systems are distributed in more than 1 plane while for the 3- to 5-membered C rings the arrangement of the ring members is in 1 plane. The relative ease of formation of the C rings is not in direct proportion to the relative stability of these rings. On the basis of their relative ease of formation the C rings may be arranged in 3 classes: 5- and 6-rings; 3-, 4- and 7-rings; 8- and higher rings. The C double bond possesses a greater ease of formation than any ring compound The ease of formation of an intramol. C-C union depends upon the relative positions of the C atoms in the chain of the starting materials; the nearer these are together, the easier the formation of the union. The C rings with a normal distribution of valences of the ring members are formed relatively more easily than the others. The relative ease of formation and the relative stability are, in several cases, further influenced by the method used in testing the stability or by the reaction used for the formation of the ring. The Th salt of glutaric acid gives no ketone. The Ca salt of adipic acid gives 43% of cyclopentanone; the Th salt, 15%; the Pb salt, 35%. The Th salt of pimelic acid gives 70-80% of cyclohexanone. The Th or Ce salt of suberic acid gives 45% of cycloheptanone. The behavior of ketones towards concentrated HCl and ThO2 is reported. Cyclopentadecane, m. 60-1°, is unchanged by heating with HI at 250° for 7 hrs. Cycloheptadecane, m. 64-5°, also is unchanged. The following figures represent d4 at t°, nD at the same temperature, MD calculated and found: Cyclopentadecane, 0.8364 at 61.5°, 1.4592, 69.26, 68.76; cycloheptadecane, 0.8239 at 73.5°, 1.4540, 78.50, 78.33; cyclododecanone, 0.9059 at 66°, 1.4571, 55.42, 54.79; cyclopentadecanone. 0.8973 at 66°, 1.4637, 69.28, 68.95; cyclohexadecanone, 0.8962 at 60°, 1.4648, 73.89, 73.48; cycloheptadecanone, 0.8830 at 70°, 1.4602, 78.51, 78.29; cyclooctadecanone, 0.8747 at 74.5°, 1.4578, 83.13, 83.04. Cyclooctanone, d474 0.9162 (d420 0.9584 (Wallach)); coefficient of expansion, 20-74°, 0.00078 per 1°. A table of densities of aliphatic and cyclic hydrocarbons at 20° is given.

IT 502-72-7, Cyclopentadecanone 830-13-7, Cyclododecanone
2550-52-9, Cyclohexadecanone
(consts. of)

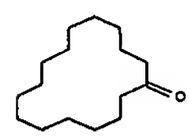
RN 502-72-7 CAPLUS
CN Cyclopentadecanone (CA INDEX NAME)



RN 830-13-7 CAPLUS
CN Cyclododecanone (CA INDEX NAME)



RN 2550-52-9 CAPLUS
CN Cyclohexadecanone (CA INDEX NAME)



L14 ANSWER 25691 OF 25691 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1926:14568 CAPLUS Full-text
DOCUMENT NUMBER: 20:14568
ORIGINAL REFERENCE NO.: 20:1791i,1792a-f
TITLE: Carbon rings. II. Synthesis of carbocyclic ketones of 10- to 18-membered rings
AUTHOR(S): Ruzicka, L.; Stoll, M.; Schinz, H.
SOURCE: Helvetica Chimica Acta (1926), 9, 249-64
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The yields of these ketones from di-CO2H acids depend upon the metal used in forming the salt; the decomposition of all of the Th salts of polymethylenedicarboxylic acids investigated yields cyclic ketones. The yield of the 9-C ring ketone was about 1.5%, the 10-C ring ketone 0.1-0.2% with decreasing yields as the number of carbons in the ring increased until the 18-C ring, where an increased yield was obtained. The cycloheptadecanone is identical with dihydrocivetone (above); the constitution of the polymethylene ketones is established by their oxidation with CrO3 to the normal polymethylenedicarboxylic acids with the same number of C atoms. All of the pure ketones with 12 or more C atoms are solids resembling camphor in appearance; the odor of the ketones with 10 to 12 C atoms is distinctly like that of camphor, the ketone with 13 C atoms has a slight cedar-wood odor as do the concentrated forms of those with more C atoms; when diluted the ketones with 14-18 C atoms have a characteristic musk odor which is most noticeable with the 15-C atom ketone. The synthesis of this type of compound opens the field for the technical preparation of natural musk and civet odorous principles and shows that the possible number of C members in a ring is much greater than was previously considered possible. Cyclodecanone (I), prepared by treating 196 g. nonane-1,9-dicarboxylic acid in warm EtOH with the calculated amount of 20% NaOH, diluting with H2O, adding 280 g. ThCl4, filtering off the separated Th salt, drying the 310 g. so obtained at 150°, distilling at 12 mm. in 4 portions from a Cu retort at increasing temperature to 500°, dissolving the distillate in Et2O, washing with NaOH and then H2O, drying over Na2SO4 and fractionally distilling at 12 mm.: (a) 50-75° (1.5 g.), (b) 75-90° (2 g.), (c) 90-105° (2.2 g.), (d) 105-20° (1.5 g.), (e) 120-40° (2.6 g.) with 36 g. residue; these fractions in MeOH were allowed to react at room temperature with semicarbazide acetate and the solns. evaporated at room temperature; fractions c and d contained the most (about 20 mg.) semicarbazone (II), m. 200-1°; when II is hydrolyzed with hot H2C2O4 solution, extracted with Et2O, washed with Na2CO3 and distilled in vacuo, I is obtained as an oil,

b12 100-2°. Oxidation of I in AcOH with CrO3 gave sebacic acid. The following cyclic ketones were obtained like I from the corresponding di-CO2H acids with one more C atom; each cyclic ketone on oxidation gave a di-CO2H acid with the same number of C atoms: cyclo-undecanone, oil, b12 110°; semicarbazone, m. 200°; cyclododecanone, m. 59°, b12 126-8°; semicarbazone, m. 220°; cyclotridecanone, m. 32°, b12 137-9°; semicarbazone, m. 200°; cyclotetradecanone m. 52°, b12 155-6°; semicarbazone, m. 195°; cyclopentadecanone or "exaltone," m. 63°, b0.3 120°; semicarbazone, m. 180°; cyclohexadecanone, m. 56°, b0.5 138°; semicarbazone, m. 180°; cycloheptadecanone, or dihydrocivetone, m. 63°, b0.3, 145°; semicarbazone, m. 191°; cyclooctadecanone, m. 71°, b0.3 157-9°.

IT 502-72-7P, Cyclopentadecanone 830-13-7P, Cyclododecanone 832-10-0P, Cyclotridecanone 2550-52-9P, Cyclohexadecanone 3603-99-4P, Cyclotetradecanone
RL: PREP (Preparation)
(preparation of)

RN 502-72-7 CAPLUS
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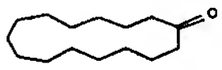

RN 830-13-7 CAPLUS
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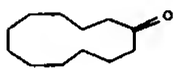

RN 832-10-0 CAPLUS
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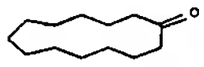
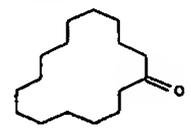


RN 2550-52-9 CAPLUS
CN Cyclohexadecanone (CA INDEX NAME)



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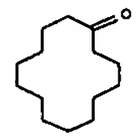

=> d his nofil

(FILE 'HOME' ENTERED AT 15:02:54 ON 05 NOV 2007)

FILE 'REGISTRY' ENTERED AT 15:03:04 ON 05 NOV 2007
L1 STR
L2 50 SEA SSS SAM L1
L3 58774 SEA ABB=ON PLU=ON C12/ESS OR C13/ESS OR C14/ESS OR C15/ESS OR C16/ESS
L*** DEL 52771 S OC11/ESS OR OC12/ESS OR OC13/ESS OR OC15/ESS
L4 53366 SEA ABB=ON PLU=ON OC11/ESS OR OC12/ESS OR OC13/ESS OR OC14/ESS OR OC15/ESS
L5 417 SEA ABB=ON PLU=ON SC11/ESS OR SC12/ESS OR SC13/ESS OR SC14/ESS OR SC15/ESS
L6 3857 SEA ABB=ON PLU=ON NC11/ESS OR NC12/ESS OR NC13/ESS OR NC14/ESS OR NC15/ESS
L7 116341 SEA ABB=ON PLU=ON (L3 OR L4 OR L5 OR L6)
L8 50 SEA SUB=L7 SSS SAM L1
L9 25195 SEA SUB=L7 SSS FUL L1

FILE 'CAPLUS' ENTERED AT 15:09:32 ON 05 NOV 2007
L10 1 SEA ABB=ON PLU=ON US200!-551152/APPS
SEL RN

FILE 'REGISTRY' ENTERED AT 15:09:48 ON 05 NOV 2007
L11 72 SEA ABB=ON PLU=ON (102029-44-7/BI OR 104923-49-1/BI OR 1119-60-4/BI OR 131685-53-5/BI OR 17325-85-8/BI OR 2066-88-8/BI OR 21430-12-6/BI OR 25118-23-4/BI OR 261631-95-2/BI OR 261631-97-4/BI OR 3112-85-4/BI OR 314245-65-3/BI OR 35000-38-5/BI OR 37031-29-1/BI OR 494834-74-1/BI OR 494834-75-2/BI OR 494834-78-5/BI OR 494834-81-0/BI OR 494834-82-1/BI OR 545339-10-4/BI OR 545339-12-6/BI OR 545339-13-7/BI OR 545339-14-8/BI OR 545339-15-9/BI OR 545339-16-0/BI OR 545339-18-2/BI OR 545339-19

-3/BI OR 545339-20-6/BI OR 545339-21-7/BI OR 663612-96-2/BI OR 663612-97-3/BI OR 663612-98-4/BI OR 663612-99-5/BI OR 663613-00-1/BI OR 663613-01-2/BI OR 663613-03-4/BI OR 663613-04-5/BI OR 663613-05-6/BI OR 663613-06-7/BI OR 663613-07-8/BI OR 663613-08-9/BI OR 663613-09-0/BI OR 663613-10-3/BI OR 663613-11-4/BI OR 663613-12-5/BI OR 663613-13-6/BI OR 663613-14-7/BI OR 663613-15-8/BI OR 663613-16-9/BI OR 663613-17-0/BI OR 663613-18-1/BI OR 663613-19-2/BI OR 68860-52-6/BI OR 72486-93-2/BI OR 74074-59-2/BI OR 756525-97-0/BI OR 760988-62-3/BI OR 760988-65-6/BI OR 760988-66-7/BI OR 760988-67-8/BI OR 760988-68-9/BI OR 760988-69-0/BI OR 760988-84-9/BI OR 760988-86-1/BI OR 760988-88-3/BI OR 760988-89-4/BI OR 760988-90-7/BI OR 760988-92-9/BI OR 760988-93-0/BI OR 773860-01-8/BI OR 821-09-0/BI OR 96-22-0/BI)
L12 21 SEA ABB=ON PLU=ON L11 AND L9

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L13 27 SEA ABB=ON PLU=ON L12
L14 25691 SEA ABB=ON PLU=ON L9

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D QUE L13
D L13 IBIB ABS HITSTR 1-27
D QUE L14
D L14 IBIB ABS HITSTR 1000-1002 20000-20002 25690-25691

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


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 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  JUL 02  LMEDLINE coverage updated
 NEWS  3  JUL 02  SCISEARCH enhanced with complete author names
 NEWS  4  JUL 02  CHEMCATS accession numbers revised
 NEWS  5  JUL 02  CA/CAplus enhanced with utility model patents from China
 NEWS  6  JUL 16  CAplus enhanced with French and German abstracts
 NEWS  7  JUL 18  CA/CAplus patent coverage enhanced
 NEWS  8  JUL 26  USPATFULL/USPAT2 enhanced with IPC reclassification
 NEWS  9  JUL 30  USGENE now available on STN
 NEWS 10  AUG 06  CAS REGISTRY enhanced with new experimental property tags
 NEWS 11  AUG 06  FSTA enhanced with new thesaurus edition
 NEWS 12  AUG 13  CA/CAplus enhanced with additional kind codes for granted
                  patents
 NEWS 13  AUG 20  CA/CAplus enhanced with CAS indexing in pre-1907 records
 NEWS 14  AUG 27  Full-text patent databases enhanced with predefined
                  patent family display formats from INPADOCDB
 NEWS 15  AUG 27  USPATOLD now available on STN
 NEWS 16  AUG 28  CAS REGISTRY enhanced with additional experimental
                  spectral property data
 NEWS 17  SEP 07  STN AnaVist, Version 2.0, now available with Derwent
                  World Patents Index
 NEWS 18  SEP 13  FORIS renamed to SOFIS
 NEWS 19  SEP 13  INPADOCDB enhanced with monthly SDI frequency
 NEWS 20  SEP 17  CA/CAplus enhanced with printed CA page images from
                  1967-1998
 NEWS 21  SEP 17  CAplus coverage extended to include traditional medicine
                  patents
 NEWS 22  SEP 24  EMBASE, EMBAL, and LEMBASE reloaded with enhancements
 NEWS 23  OCT 02  CA/CAplus enhanced with pre-1907 records from Chemisches
                  Zentralblatt
 NEWS 24  OCT 19  BEILSTEIN updated with new compounds

 NEWS EXPRESS  19 SEPTEMBER 2007:  CURRENT WINDOWS VERSION IS V8.2,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 11:36:54 ON 08 NOV 2007

=> file reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.21       0.21

FILE 'REGISTRY' ENTERED AT 11:37:17 ON 08 NOV 2007
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provided by InfoChem.

STRUCTURE FILE UPDATES:     7 NOV 2007  HIGHEST RN 952647-77-7
DICTIONARY FILE UPDATES:    7 NOV 2007  HIGHEST RN 952647-77-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10.551152\elected spec.str
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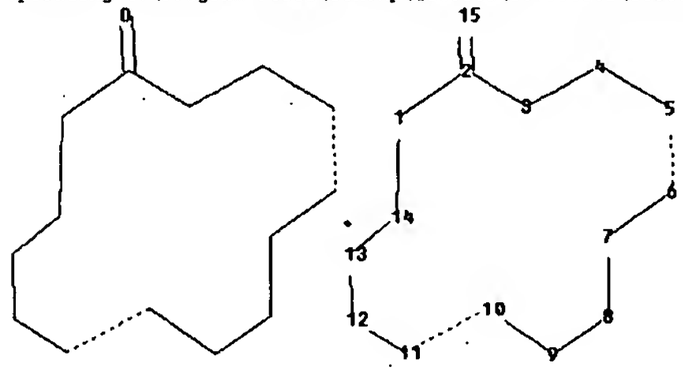


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ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14
chain bonds :
2-15
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ring bonds :
1-2  1-14  2-3  3-4  4-5  5-6  6-7  7-8  8-9  9-10  10-11  11-12  12-13  13-14
exact/norm bonds :
1-2  1-14  2-3  2-15  3-4  4-5  5-6  6-7  7-8  8-9  9-10  10-11  11-12  12-13  13-14


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:CLASS


L1      STRUCTURE UPLOADED

=>

=> d
L1 HAS NO ANSWERS
L1                STR
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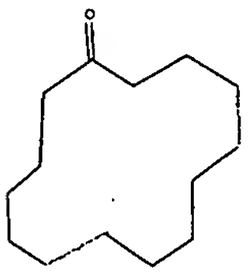


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Structure attributes must be viewed using STN Express query preparation.


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SAMPLE SCREEN SEARCH COMPLETED -   505209 TO ITERATE

  0.4% PROCESSED     2000 ITERATIONS                              28 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:     10063920 TO 10144440
PROJECTED ANSWERS:          136416 TO   146500

L2            28 SEA SSS SAM L1

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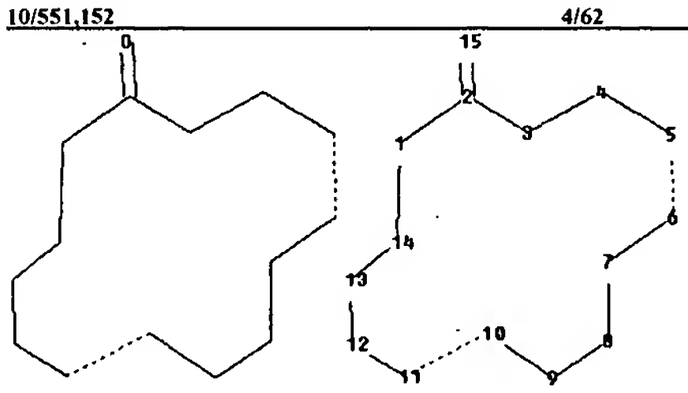


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ring nodes :
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chain bonds :
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ring bonds :
1-2  1-14  2-3  3-4  4-5  5-6  6-7  7-8  8-9  9-10  10-11  11-12  12-13  13-14
exact/norm bonds :
2-15  5-6  10-11
exact bonds :
1-2  1-14  2-3  3-4  4-5  6-7  7-8  8-9  9-10  11-12  12-13  13-14
isolated ring systems :
containing 1 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:CLASS


L3      STRUCTURE UPLOADED

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L3 HAS NO ANSWERS
L3                STR
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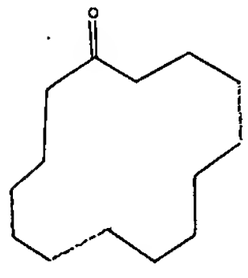

Structure attributes must be viewed using STN Express query preparation.

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4.5% PROCESSED 2000 ITERATIONS 1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 881893 TO 907147
PROJECTED ANSWERS: 164 TO 730

L4 1 SEA SSS SAM L3

=> screen 1139
L5 SCREEN CREATED

=> s l5 and l4 sss sam
L4 MAY NOT BE USED HERE
The L-number entered was not created by a STRUCTURE or SCREEN command.

=> s l5 and l3 sss sam
SAMPLE SEARCH INITIATED 11:40:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 15947 TO ITERATE

12.5% PROCESSED 2000 ITERATIONS 3 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

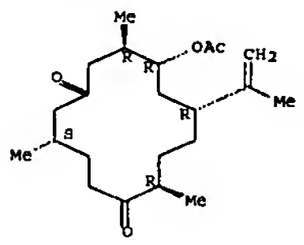
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 311377 TO 326503
PROJECTED ANSWERS: 185 TO 771

L6 3 SEA SSS SAM L5 AND L3

=> d scan

L6 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,6-Cyclotetradecanedione, 12-(acetyloxy)-3,7,13-trimethyl-10-(1-methylethenyl)-, [3S-(3R*,7S*,10S*,12S*,13S*)]- (9CI)
MF C22 H36 O4

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>
Connection closed by remote host

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Welcome to STN International! Enter x:x

LOGINID:SSPTARHH1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 JUL 02 LMEDLINE coverage updated
NEWS 3 JUL 02 SCISEARCH enhanced with complete author names
NEWS 4 JUL 02 CHEMCATS accession numbers revised
NEWS 5 JUL 02 CA/CAplus enhanced with utility model patents from China
NEWS 6 JUL 16 CAplus enhanced with French and German abstracts
NEWS 7 JUL 18 CA/CAplus patent coverage enhanced
NEWS 8 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 9 JUL 30 USGENE now available on STN
NEWS 10 AUG 06 CAS REGISTRY enhanced with new experimental property tags
NEWS 11 AUG 06 FSTA enhanced with new thesaurus edition
NEWS 12 AUG 13 CA/CAplus enhanced with additional kind codes for granted patents
NEWS 13 AUG 20 CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 14 AUG 27 Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 15 AUG 27 USPATOLD now available on STN
NEWS 16 AUG 28 CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 17 SEP 07 STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 18 SEP 13 FORIS renamed to SOFIS
NEWS 19 SEP 13 INPADOCDB enhanced with monthly SDI frequency

NEWS 20 SEP 17 CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 21 SEP 17 CAplus coverage extended to include traditional medicine patents
NEWS 22 SEP 24 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 23 OCT 02 CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 24 OCT 19 BEILSTEIN updated with new compounds

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:02:54 ON 08 NOV 2007

=> log hold
COST IN U.S. DOLLARS SINCE FILE ENTRY 0.21 TOTAL SESSION 0.21

FULL ESTIMATED COST

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 13:03:37 ON 08 NOV 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTARHH1626

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'HOME' AT 13:04:06 ON 08 NOV 2007
FILE 'HOME' ENTERED AT 13:04:06 ON 08 NOV 2007

COST IN U.S. DOLLARS SINCE FILE ENTRY 0.21 TOTAL SESSION 0.21

FULL ESTIMATED COST

=>
=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY 0.21 TOTAL SESSION 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 13:04:11 ON 08 NOV 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 NOV 2007 HIGHEST RN 952647-77-7
DICTIONARY FILE UPDATES: 7 NOV 2007 HIGHEST RN 952647-77-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

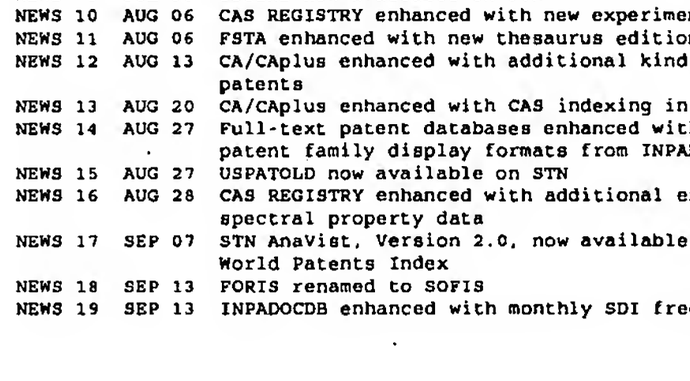
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10.551152\elected spec 2.str

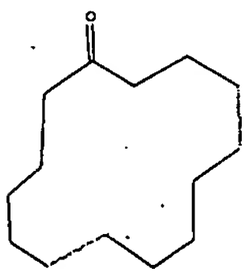


chain nodes :
15
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14
chain bonds :
2-15
ring bonds :
1-2 1-14 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14
exact/norm bonds :
2-15 5-6 10-11
exact bonds :
1-2 1-14 2-3 3-4 4-5 6-7 7-8 8-9 9-10 11-12 12-13 13-14
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS

```
L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR
```



```
Structure attributes must be viewed using STN Express query preparation.

=> screen 13
L2    SCREEN CREATED

=> s l2 and l1 sss sam
SAMPLE SEARCH INITIATED 13:12:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     44726 TO ITERATE

  4.5% PROCESSED     2000 ITERATIONS                          1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      881893 TO   907147
PROJECTED ANSWERS:            164 TO      730

L3            1 SEA SSS SAM L2 AND L1

=> screen 1139
L4    SCREEN CREATED

=> s l2 and l4 and l1 sss sam
SAMPLE SEARCH INITIATED 13:13:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     15947 TO ITERATE

 12.5% PROCESSED     2000 ITERATIONS                          3 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      311377 TO   326503
PROJECTED ANSWERS:            185 TO      771
```



```
L5            3 SEA SSS SAM L2 AND L4 AND L1

=> screen 1138
L6    SCREEN CREATED

=> s l2 and l4 and l6 and l1 sss sam
SAMPLE SEARCH INITIATED 13:14:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     10426 TO ITERATE

 19.2% PROCESSED     2000 ITERATIONS                          0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.02

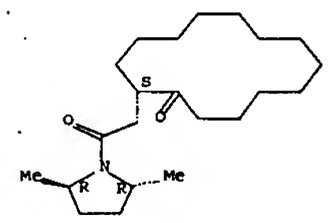
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      202401 TO   214639
PROJECTED ANSWERS:              0 TO        0

L7            0 SEA SSS SAM L2 AND L4 AND L6 AND L1

=> d l5 scan

L5   3 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   Pyrrolidine, 2,5-dimethyl-1-[(2-oxocyclotetradecyl)acetyl]-,
     (2R-[1(S*),2α,5β])- (9CI)
MF   C22 H39 N O2

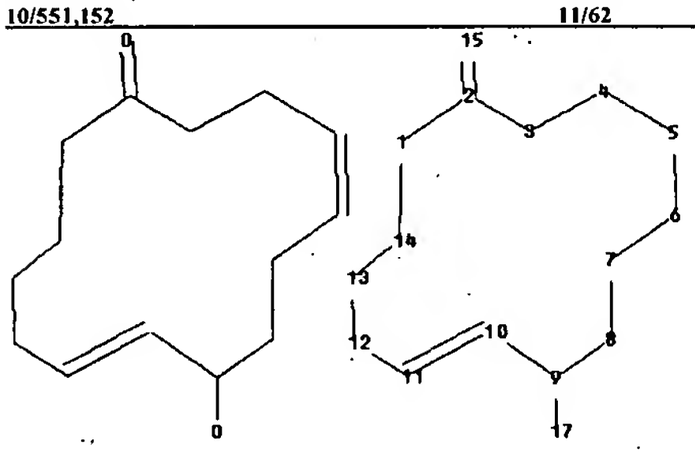
Absolute stereochemistry.
```



```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>
Uploading C:\Program Files\Stnexp\Queries\10.551152\specific species.str
```

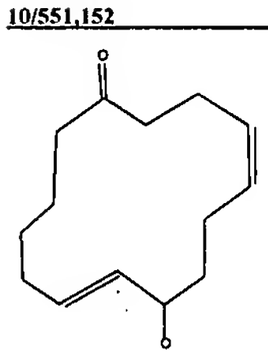



```
chain nodes :
15  17
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14
chain bonds :
2-15  9-17
ring bonds :
1-2  1-14  2-3  3-4  4-5  5-6  6-7  7-8  8-9  9-10  10-11  11-12  12-13  13-14
exact/norm bonds :
2-15  9-17
exact bonds :
1-2  1-14  2-3  3-4  4-5  5-6  6-7  7-8  8-9  9-10  10-11  11-12  12-13  13-14
isolated ring systems :
containing 1 :

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:CLASS  17:CLASS

L8      STRUCTURE UPLOADED

=> d
L8 HAS NO ANSWERS
L8              STR
```

```
Structure attributes must be viewed using STN Express query preparation.

=> s l8 sss sam
SAMPLE SEARCH INITIATED 13:16:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      5084 TO ITERATE

 39.3% PROCESSED     2000 ITERATIONS                          0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       97405 TO   105955
PROJECTED ANSWERS:              0 TO        0

L9            0 SEA SSS SAM L8

=> d hist

     (FILE 'HOME' ENTERED AT 13:02:54 ON 08 NOV 2007)

     FILE 'REGISTRY' ENTERED AT 13:04:11 ON 08 NOV 2007
L1              STRUCTURE UPLOADED
L2              SCREEN 13
L3            1 S L2 AND L1 SSS SAM
L4              SCREEN 1139
L5            3 S L2 AND L4 AND L1 SSS SAM
L6              SCREEN 1138
L7            0 S L2 AND L4 AND L6 AND L1 SSS SAM
L8              STRUCTURE UPLOADED
L9            0 S L8 SSS SAM

=> s l4 and l8 sss sam
SAMPLE SEARCH INITIATED 13:17:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      3277 TO ITERATE

 61.0% PROCESSED     2000 ITERATIONS                          0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       62107 TO    68973
```

```
PROJECTED ANSWERS:                0 TO        0

L10           0 SEA SSS SAM L4 AND L8

=> s 14 and 16 and 18 sss sam
SAMPLE SEARCH INITIATED 13:17:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      2540 TO ITERATE

 78.7% PROCESSED      2000 ITERATIONS                          0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          47777 TO     53823
PROJECTED ANSWERS:                0 TO         0

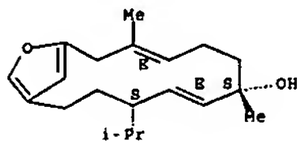
L11           0 SEA SSS SAM L4 AND L6 AND L8

=> s C14/ess
L12        5360 C14/ESS

=> d scan

L12  5360 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   14-Oxabicyclo[11.2.1]hexadeca-5,10,13(16),15-tetraen-7-ol,
     7,11-dimethyl-4-(1-methylethyl)-, (4S,5E,7S,10E)-
MF   C20 H30 O2

Absolute stereochemistry.  Rotation (-).
Double bond geometry as shown.
```




```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l8 sub=l12 sss sam
SAMPLE SUBSET SEARCH INITIATED 13:19:59 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -       28 TO ITERATE

100.0% PROCESSED       28 ITERATIONS                     0 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):       ONLINE  **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):        243 TO       877
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):             0 TO         0

L13           0 SEA SUB=L12 SSS SAM L8
```



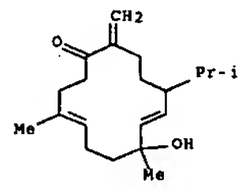
```
=> s l8 sub=l12 sss full
FULL SUBSET SEARCH INITIATED 13:20:06 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -      511 TO ITERATE

100.0% PROCESSED      511 ITERATIONS                     5 ANSWERS
SEARCH TIME: 00.00.01

L14           5 SEA SUB=L12 SSS FUL L8

=> d scan

L14  5 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4,9-Cyclotetradecadien-1-one, 8-hydroxy-4,8-dimethyl-14-methylene-11-(1-
     methylethyl)-, [8R-(4E,8R*,9E,11S*)]- (9CI)
MF   C20 H32 O2
```

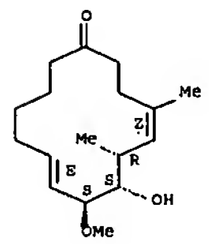



```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

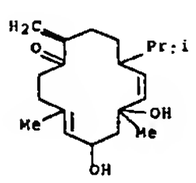
L14  5 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-,
     (4Z,6R,7S,8S,9E)-
MF   C17 H28 O3

Absolute stereochemistry.  Rotation (+).
Double bond geometry as shown.
```




```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L14  5 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4,9-Cyclotetradecadien-1-one, 6,8-dihydroxy-4,8-dimethyl-14-methylene-11-
     (1-methylethyl)-, [6R-(4E,6R*,8S*,9E,11S*)]- (9CI)
MF   C20 H32 O3
```

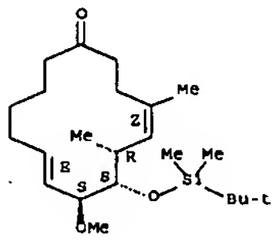



```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

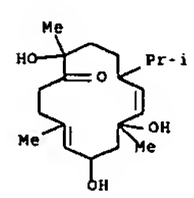
L14  5 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4,9-Cyclotetradecadien-1-one, 7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-
     methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)-
MF   C23 H42 O3 Si

Absolute stereochemistry.
Double bond geometry as shown.
```




```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L14  5 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4,9-Cyclotetradecadien-1-one, 6,8,14-trihydroxy-4,8,14-trimethyl-11-(1-
     methylethyl)- (9CI)
MF   C20 H34 O4
```


```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

ALL ANSWERS HAVE BEEN SCANNED

=> d hist

     (FILE 'HOME' ENTERED AT 13:02:54 ON 08 NOV 2007)

     FILE 'REGISTRY' ENTERED AT 13:04:11 ON 08 NOV 2007
L1             STRUCTURE UPLOADED
L2             SCREEN 13
L3           1 S L2 AND L1 SSS SAM
L4             SCREEN 1139
L5           3 S L2 AND L4 AND L1 SSS SAM
L6             SCREEN 1138
L7           0 S L2 AND L4 AND L6 AND L1 SSS SAM
L8             STRUCTURE UPLOADED
L9           0 S L8 SSS SAM
L10          0 S L4 AND L8 SSS SAM
L11          0 S L4 AND L6 AND L8 SSS SAM
L12       5360 S C14/ESS
L13          0 S L8 SSS SAM SUB=L12
L14          5 S L8 SSS FULL SUB=L12

=> s C12/ESS OR C13/ESS OR                C14/ESS OR C15/ESS OR C16/ESS
       21130 C12/ESS
        2632 C13/ESS
        5360 C14/ESS
        2353 C15/ESS
       27476 C16/ESS
L15    58806 C12/ESS OR C13/ESS OR          C14/ESS OR C15/ESS OR
             C16/ESS

=> s OC11/ESS OR OC12/ESS OR              OC13/ESS OR OC14/ESS OR OC15/ESS
        3447 OC11/ESS
        1401 OC12/ESS
       24988 OC13/ESS
         598 OC14/ESS
       22980 OC15/ESS
L16    53391 OC11/ESS OR OC12/ESS OR              OC13/ESS OR OC14/ESS OR
             OC15/ESS

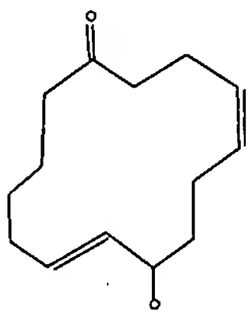
=> s SC11/ESS OR SC12/ESS OR              SC13/ESS OR SC14/ESS OR SC15/ESS
          86 SC11/ESS
          90 SC12/ESS
          96 SC13/ESS
```

```
            69 SC14/ESS
            76 SC15/ESS
L17        417 SC11/ESS OR SC12/ESS OR                SC13/ESS OR SC14/ESS OR
               SC15/ESS

=> s NC11/ESS OR NC12/ESS OR                NC13/ESS OR NC14/ESS OR NC15/ESS
           336 NC11/ESS
          2015 NC12/ESS
           583 NC13/ESS
           225 NC14/ESS
           726 NC15/ESS
L18       3857 NC11/ESS OR NC12/ESS OR                NC13/ESS OR NC14/ESS OR
               NC15/ESS

=> s l15 or l16 or l17 or l18
         18531 l18
L19     131063 L15 OR L16 OR L17 OR l18

=> d l8
L8 HAS NO ANSWERS
L8                STR
```



```
Structure attributes must be viewed using STN Express query preparation.

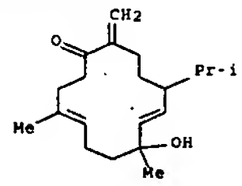
=> s sub=l19 sss full l8
FULL SUBSET SEARCH INITIATED 13:39:32 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -     15151 TO ITERATE

100.0% PROCESSED     15151 ITERATIONS                                5 ANSWERS
SEARCH TIME: 00.00.01

L20             5 SEA SUB=L19 SSS FUL L8

=> d scan

L20  5 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4,9-Cyclotetradecadien-1-one, 8-hydroxy-4,8-dimethyl-14-methylene-11-(1-
     methylethyl)-, [8R-(4E,8R*,9E,11S*)]- (9CI)
MF   C20 H32 O2
```

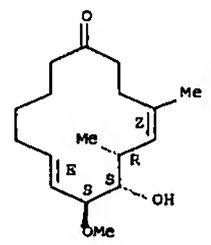



```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

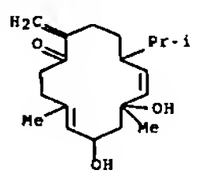
L20  5 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4,9-Cyclotetradecadien-1-one, 7-hydroxy-8-methoxy-4,6-dimethyl-,
     (4Z,6R,7S,8S,9E)-
MF   C17 H28 O3

Absolute stereochemistry.  Rotation (+).
Double bond geometry as shown.
```



```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L20  5 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4,9-Cyclotetradecadien-1-one, 6,8-dihydroxy-4,8-dimethyl-14-methylene-11-
     (1-methylethyl)-, [6R-(4E,6R*,8S*,9E,11S*)]- (9CI)
MF   C20 H32 O3
```

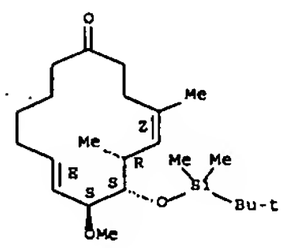



```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

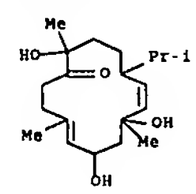
L20  5 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4,9-Cyclotetradecadien-1-one, 7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-
     methoxy-4,6-dimethyl-, (4Z,6R,7S,8S,9E)-
MF   C23 H42 O3 Si

Absolute stereochemistry.
Double bond geometry as shown.
```



```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L20  5 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4,9-Cyclotetradecadien-1-one, 6,8,14-trihydroxy-4,8,14-trimethyl-11-(1-
     methylethyl)- (9CI)
MF   C20 H34 O4
```

```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                              ENTRY      SESSION
FULL ESTIMATED COST                          479.20      479.41

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FILE LAST UPDATED: 7 Nov 2007  (20071107/ED)

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L21          10 L20

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L21  ANSWER 1 OF 10  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:        2006:10861  CAPLUS  Full-text
DOCUMENT NUMBER:         144:88082
TITLE:                   Preparation of migrastatin and its analogs for use in
                         pharmaceutical compositions for the treatment of
                         cancer
INVENTOR(S):             Danishefsky, Samuel J.; Gaul, Christoph; Njardarson,
                         Jon T.; Moore, Malcolm  A. S.; Wu, Kaida; Dorn, David
                         C.; Mandal, Mihirbaran
PATENT ASSIGNEE(S):      Sloan-Kettering Institute for Cancer Research, USA
```

SOURCE: PCT Int. Appl., 266 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006001967	A2	20060105	WO 2005-US18603	20050525
WO 2006001967	A3	20060727		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
CA 2582766	A1	20060330	CA 2005-2582766	20050923
WO 2006034478	A2	20060330	WO 2005-US34305	20050923
WO 2006034478	A3	20061130		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1805161	A2	20070711	EP 2005-800816	20050923
PRIORITY APPLN. INFO.:			US 2004-574114P	P 20040525
			US 2004-612415P	P 20040923
			WO 2005-US18603	A 20050525
			WO 2005-US34305	W 20050923
OTHER SOURCE(S):			MARPAT 144:88082	

L21 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:247346 CAPLUS Full-text
DOCUMENT NUMBER: 142:403680
TITLE: Synthetic analogues of migrastatin that inhibit mammary tumor metastasis in mice
AUTHOR(S): Shan, Dandan; Chen, Lin; Njardarson, Jon T.; Gaul, Christoph; Ma, Xiaojing; Danishefsky, Samuel J.; Huang, Xin-Yun
CORPORATE SOURCE: Department of Physiology, Weill Medical College of Cornell University, New York, NY, 10021, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2005), 102(10), 3772-3776
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:182633 CAPLUS Full-text
DOCUMENT NUMBER: 142:279984
TITLE: Preparation of migrastatin analogs as cell migration inhibitors
INVENTOR(S): Huang, Xin-Yun
PATENT ASSIGNEE(S): Cornell Research Foundation, Inc., USA
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005019181	A1	20050303	WO 2004-US9211	20040325
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			US 2003-496165P	P 20030819
OTHER SOURCE(S):			CASREACT 142:279984; MARPAT 142:279984	
REFERENCE COUNT:			3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT	

L21 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:857572 CAPLUS Full-text
DOCUMENT NUMBER: 141:331967
TITLE: Preparation of migrastatin analogs and their biological activity
INVENTOR(S): Danishefsky, Samuel J.; Gaul, Christoph; Njardarson, Jon T.
PATENT ASSIGNEE(S): Sloan-Kettering Institute for Cancer Research, USA
SOURCE: PCT Int. Appl., 254 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087673	A2	20041014	WO 2004-US9571	20040326
WO 2004087673	A3	20041104		
WO 2004087673	B1	20050310		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,				

SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2520732	A1	20041014	CA 2004-2520732	20040326
EP 1613603	A2	20060111	EP 2004-758529	20040326
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
JP 2006521407	T	20060921	JP 2006-509430	20040326
US 2007037852	A1	20070215	US 2006-551158	20060925
PRIORITY APPLN. INFO.:			US 2003-458827P	P 20030328
			US 2003-496165P	P 20030819
			WO 2004-US9571	W 20040326
OTHER SOURCE(S):			CASREACT 141:331967; MARPAT 141:331967	

L21 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:857571 CAPLUS Full-text
DOCUMENT NUMBER: 141:349965
TITLE: Preparation of migrastatin analogs and their biological activity
INVENTOR(S): Huang, Xin-Yun; Danishefsky, Samuel J.; Gaul, Christoph; Njardarson, Jon T.
PATENT ASSIGNEE(S): Cornell Research Foundation, Inc., USA; Sloan-Kettering Institute for Cancer Research
SOURCE: PCT Int. Appl., 268 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087672	A1	20041014	WO 2004-US9380	20040326
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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CA 2520377	A1	20041014	CA 2004-2520377	20040326
EP 1608626	A1	20051228	EP 2004-758436	20040326
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
JP 2006523233	T	20061012	JP 2006-509369	20040326
US 2007037783	A1	20070215	US 2006-551152	20060925
PRIORITY APPLN. INFO.:			US 2003-458827P	P 20030328
			US 2003-496165P	P 20030819
			WO 2004-US9380	W 20040326
OTHER SOURCE(S):			CASREACT 141:349965; MARPAT 141:349965	
REFERENCE COUNT:			6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT	

L21 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:607055 CAPLUS Full-text
DOCUMENT NUMBER: 141:295757
TITLE: The Migrastatin family: discovery of potent cell migration inhibitors by chemical synthesis
AUTHOR(S): Gaul, Christoph; Njardarson, Jon T.; Shan, Dandan; Dorn, David C.; Wu, Kai-Da; Tong, William P.; Huang,

Xin-Yun; Moore, Malcolm A. S.; Danishefsky, Samuel J.
CORPORATE SOURCE: Laboratory for Bioorganic Chemistry, Sloan-Kettering Institute for Cancer Research, New York, OR, 10021, USA
SOURCE: Journal of the American Chemical Society (2004), 126(36), 11326-11337
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:295757
REFERENCE COUNT: 108 THERE ARE 108 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:8166 CAPLUS Full-text
DOCUMENT NUMBER: 140:199127
TITLE: Discovery of Potent Cell Migration Inhibitors through Total Synthesis: Lessons from Structure-Activity Studies of (+)-Migrastatin
AUTHOR(S): Njardarson, Jon T.; Gaul, Christoph; Shan, Dandan; Huang, Xin-Yun; Danishefsky, Samuel J.
CORPORATE SOURCE: Laboratory for Bioorganic Chemistry, Sloan-Kettering Institute for Cancer Research, New York, NY, 10021, USA
SOURCE: Journal of the American Chemical Society (2004), 126(4), 1038-1040
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:199127
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:129084 CAPLUS Full-text
DOCUMENT NUMBER: 102:129084
TITLE: A new cembranoid from tobacco, IV
AUTHOR(S): Sinnwell, Volker; Heemann, Volker; Bylov, Anne Marie; Hass, Werner; Kahre, Claudius; Seehofer, Friedlieb
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Hamburg, Hamburg, 2000/13, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1984), 39C(11-12), 1023-6
CODEN: ZNCBDA; ISSN: 0341-0382
DOCUMENT TYPE: Journal
LANGUAGE: English

L21 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:435859 CAPLUS Full-text
DOCUMENT NUMBER: 101:35859
TITLE: Application of 2D-NMR spectroscopy in the structural determination of a new tobacco cembranoid
AUTHOR(S): Nishida, Toshiaki; Wahlberg, Inger; Nordfors, Kerstin; Vogt, Carmen; Enzell, Curt R.
CORPORATE SOURCE: Res. Dep., Swedish Tobacco Co., Stockholm, S-104 62, Swed.
SOURCE: Tetrahedron Letters (1984), 25(12), 1299-302
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English

L21 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:423762 CAPLUS Full-text
DOCUMENT NUMBER: 101:23762
TITLE: Photosensitized oxidation of isocembrol. VII. Products of reaction at the C11 double bond
AUTHOR(S): Paldygin, V. A.; Pleshkov, I. G.; Gatilov, Yu. V.; Yaroshenko, N. I.; Salenko, V. L.; Shevtsov, S. A.; Pentegova, V. A.
CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR
SOURCE: Khimiya Prirodnykh Soedinenii (1984), (1), 48-56
CODEN: KPSUAR; ISSN: 0023-1150
DOCUMENT TYPE: Journal
LANGUAGE: Russian

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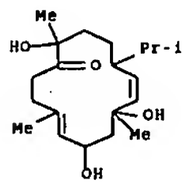
L21 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:129084 CAPLUS Full-text
DOCUMENT NUMBER: 102:129084
TITLE: A new cembranoid from tobacco, IV
AUTHOR(S): Sinnwell, Volker; Heemann, Volker; Bylov, Anne Marie; Hass, Werner; Kahre, Claudius; Seehofer, Friedlieb
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Hamburg, Hamburg, 2000/13, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1984), 39C(11-12), 1023-6
CODEN: ZNCBDA; ISSN: 0341-0382
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 4,8-Dimethyl-11-isopropyl-6,8-dihydroxypentadeca-4,9-dien-14-on-1-al (I) was identified as a new natural product from tobacco. I was isolated from the surface gum of fresh tobacco. The spectral data, chemical properties, and the synthesis of I are given. I undergoes self-degradation to norditerpenoids.

IT 95360-15-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and glycolic cleavage of)

RN 95360-15-9 CAPLUS

CN 4,9-Cyclotetradecadien-1-one, 6,8,14-trihydroxy-4,8,14-trimethyl-11-(1-methylethyl)- (9CI) (CA INDEX NAME)



L21 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:435859 CAPLUS Full-text
DOCUMENT NUMBER: 101:35859
TITLE: Application of 2D-NMR spectroscopy in the structural determination of a new tobacco cembranoid
AUTHOR(S): Nishida, Toshiaki; Wahlberg, Inger; Nordfors, Kerstin;

Vogt, Carmen; Enzell, Curt R.
CORPORATE SOURCE: Res. Dep., Swedish Tobacco Co., Stockholm, S-104 62, Swed.
SOURCE: Tetrahedron Letters (1984), 25(12), 1299-302
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
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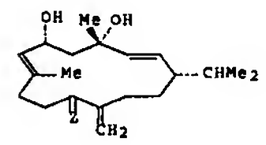


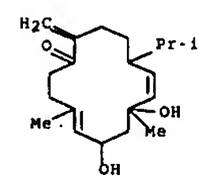
I

AB A new cembranoid was isolated from the flowers of Greek tobacco and its structure determined to be I (Z = O) by 2D-NMR and by synthesis from the hydroperoxide I (Z = α-HOO, β-H).

IT 90660-18-7
RL: BIOL (Biological study)
(from tobacco, structure of)

RN 90660-18-7 CAPLUS

CN 4,9-Cyclotetradecadien-1-one, 6,8-dihydroxy-4,8-dimethyl-14-methylene-11-(1-methylethyl)-, [6R-(4E,6R*,8S*,9E,11S*)]- (9CI) (CA INDEX NAME)



L21 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:423762 CAPLUS Full-text
DOCUMENT NUMBER: 101:23762
TITLE: Photosensitized oxidation of isocembrol. VII. Products of reaction at the C11 double bond
AUTHOR(S): Paldygin, V. A.; Pleshkov, I. G.; Gatilov, Yu. V.; Yaroshenko, N. I.; Salenko, V. L.; Shevtsov, S. A.; Pentegova, V. A.
CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR
SOURCE: Khimiya Prirodnykh Soedinenii (1984), (1), 48-56
CODEN: KPSUAR; ISSN: 0023-1150
DOCUMENT TYPE: Journal
LANGUAGE: Russian
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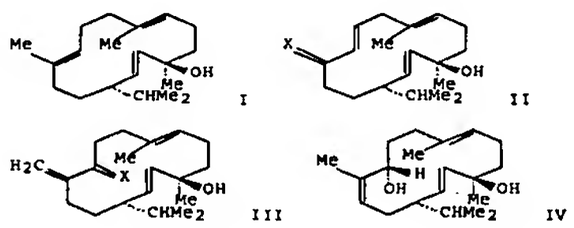


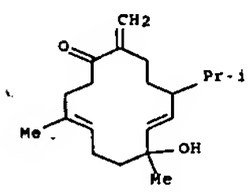
I II III IV

AB Photochem. oxidation of isocembrol (I) yielded reaction products derived from attack at the C-11 double bond and gave a mixture containing diols II (X = α-OH, β-Me; α-Me, β-OH), III (X = α-H, β-OH; α-OH, β-H) and IV. The structure of diol II (X = α-OH, β-Me) was confirmed by x-ray crystallog.

IT 90659-77-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 90659-77-1 CAPLUS

CN 4,9-Cyclotetradecadien-1-one, 8-hydroxy-4,8-dimethyl-14-methylene-11-(1-methylethyl)-, [8R-(4E,8R*,9E,11S*)]- (9CI) (CA INDEX NAME)



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DICTIONARY FILE UPDATES: 7 NOV 2007 HIGHEST RN 952647-77-7

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http://www.cas.org/support/stngen/stndoc/properties.html

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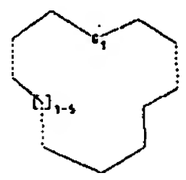
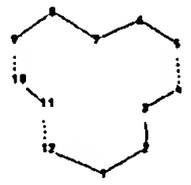




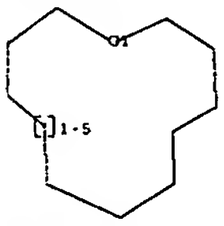
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
ring bonds :
1-2 1-12 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-12 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 :

G1:C,O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom

L22 STRUCTURE UPLOADED

=> d
L22 HAS NO ANSWERS
L22 STR



G1 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

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=> s sub=l19 sss full l22
FULL SUBSET SEARCH INITIATED 13:44:52 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -    113851 TO ITERATE

100.0% PROCESSED    113851 ITERATIONS                      20708 ANSWERS
SEARCH TIME: 00.00.02

L23        20708 SEA SUB=L19 SSS FUL L22

=> screen l1139
'LL13' NOT A SCREEN NUMBER
The number entered is not a CAS ONLINE screen number.
Screen numbers are listed in the CAS ONLINE Screen Dictionary,
a printed document.

=> screen 1139
'L999' NOT A SCREEN NUMBER
The number entered is not a CAS ONLINE screen number.
Screen numbers are listed in the CAS ONLINE Screen Dictionary,
a printed document.

=> screen 1139
L24    SCREEN CREATED

=> s l24 and l23
L23 MAY NOT BE USED HERE
The L-number entered was not created by a STRUCTURE or SCREEN command.

=> s l24 sub=l23
ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):full
FULL SUBSET SEARCH INITIATED 13:45:47 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED                    7017 ANSWERS
SEARCH TIME: 00.00.01

L25         7017 SEA SUB=L23 SSS FUL L24

=> d hist

     (FILE 'HOME' ENTERED AT 13:02:54 ON 08 NOV 2007)

     FILE 'REGISTRY' ENTERED AT 13:04:11 ON 08 NOV 2007
L1              STRUCTURE UPLOADED
L2              SCREEN 13
```



```
L3              1 S L2 AND L1 SSS SAM
L4                SCREEN 1139
L5              3 S L2 AND L4 AND L1 SSS SAM
L6                SCREEN 1138
L7              0 S L2 AND L4 AND L6 AND L1 SSS SAM
L8                STRUCTURE UPLOADED
L9              0 S L8 SSS SAM
L10             0 S L4 AND L8 SSS SAM
L11             0 S L4 AND L6 AND L8 SSS SAM
L12          5360 S C14/ESS
L13             0 S L8 SSS SAM SUB=L12
L14             5 S L8 SSS FULL SUB=L12
L15         58806 S C12/ESS OR C13/ESS OR                C14/ESS OR C15/ESS OR C
L16         53391 S OC11/ESS OR OC12/ESS OR                OC13/ESS OR OC14/ESS
L17           417 S SC11/ESS OR SC12/ESS OR                SC13/ESS OR SC14/ESS
L18          3857 S NC11/ESS OR NC12/ESS OR                NC13/ESS OR NC14/ESS
L19        131063 S L15 OR L16 OR L17 OR L18
L20             5 S SSS FULL L8 SUB=L19

     FILE 'CAPLUS' ENTERED AT 13:40:02 ON 08 NOV 2007
L21            10 S L20

     FILE 'REGISTRY' ENTERED AT 13:44:15 ON 08 NOV 2007
L22               STRUCTURE UPLOADED
L23         20708 S SSS FULL L22 SUB=L19
L24               SCREEN 1139
L25          7017 S L24  SUB=L23 FULL

=> d l1
L1 HAS NO ANSWERS
L1                STR
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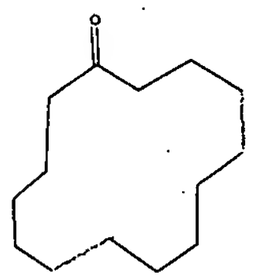

Structure attributes must be viewed using STN Express query preparation.

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FULL SUBSET SEARCH INITIATED 13:46:53 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -     57171 TO ITERATE

100.0% PROCESSED     57171 ITERATIONS                      180 ANSWERS
SEARCH TIME: 00.00.01

L26           180 SEA SUB=L19 SSS FUL L1

=> d scan
```
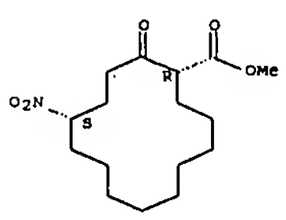



```
L26  180 ANSWERS    REGISTRY  COPYRIGHT 2007 ACS on STN
IN   Cyclotetradecanecarboxylic acid, 5-nitro-2-oxo-, methyl ester, (1R*,5S*)-
     (9CI)
MF   C16 H27 N O5

Relative stereochemistry.
```

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              386.20     896.51

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                 ENTRY    SESSION
CA SUBSCRIBER PRICE                               0.00      -2.34

FILE 'CAPLUS' ENTERED AT 13:47:07 ON 08 NOV 2007
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FILE LAST UPDATED: 7 Nov 2007  (20071107/ED)

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http://www.cas.org/infopolicy.html

=> s l26
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L27             241 L26

=> d cost
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
CONNECT CHARGES                                    0.41      28.78
NETWORK CHARGES                                    0.06       4.44
SEARCH CHARGES                                     0.00     836.15
DISPLAY CHARGES                                    0.00      27.61
                                                -------   -------
FULL ESTIMATED COST                                0.47     896.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                 ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00      -2.34

IN FILE 'CAPLUS' AT 13:47:17 ON 08 NOV 2007

=>
=> s l27 and py<2003
      22908272 PY<2003
L28           212 L27 AND PY<2003

=> d ibib abs hitstr 1-10

L28  ANSWER 1 OF 212  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2003:757086  CAPLUS  Full-text
DOCUMENT NUMBER:          139:260377
TITLE:                    Method of controlling release of bitterness inhibitors
                          in chewing gum, and gum produced thereby
INVENTOR(S):              Gudas, Victor V.; Reed, Michael A.; Schnell, Philip
                          G.; Tyrpin, Henry T.; Witkewitz, David L.; Greenberg,
                          Michael J.; Wolf, Fred R.
PATENT ASSIGNEE(S):       USA
SOURCE:                   U.S. Pat. Appl. Publ., 15 pp., Cont.-in-part of U.S.
                          Ser. No. 621,780.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   22
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    -------------------      --------
     US 2003180414         A1    20030925    US 2002-280688           20021025
     CA 2271889            A1    19980604    CA 1996-2271889          19961127 <--
     CA 2271889            C     20040127
     CA 2431848            A1    19980604    CA 1996-2431848          19961127 <--
     CA 2431848            C     20070717
     CA 2431856            A1    19980604    CA 1996-2431856          19961127 <--
     WO 9823165            A1    19980604    WO 1996-US18977          19961127 <--
         W:  AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT,
             RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN
         RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
             IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG
     AU 9712745            A     19980622    AU 1997-12745            19961127 <--
     EP 969733             A1    20000112    EP 1996-943523           19961127 <--
     EP 969733             B1    20060621
         R:  DE, FR, GB
     CA 2272703            A1    19980604    CA 1996-2272703          19961223 <--
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CA 2272703	C	20020924			
CA 2273034	A1	19980604	CA 1996-2273034	19961223	<--
CA 2273034	C	20020917			
WO 9823166	A1	19980604	WO 1996-US20252.	19961223	<--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN					
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG					
AU 9713382	A	19980622	AU 1997-13382	19961223	<--
AU 9717432	A	19980622	AU 1997-17432	19961223	<--
AU 719781	B2	20000518			
EP 967883	A1	20000105	EP 1996-945948	19961223	<--
EP 967883	B1	20030924			
R: DE, DK, FR, GB					
EP 979039	A1	20000216	EP 1996-944881	19961223	<--
EP 979039	B1	20070307			
R: DE, FR, GB					
US 6472000	B1	20021029	US 1999-319054	19990526	<--
WO 2000035298	A1	20000622	WO 1999-US29792	19991214	<--
W: US					
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
US 6949264	B1	20050927	US 2000-621780	20000721	
EP 1347746	A1	20031001	EP 2001-953503	20010717	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
AU 773949	B2	20040610	AU 2002-23197	20020308	
AU 2004233478	A1	20041223	AU 2004-233478	20041125	
AU 2004233478	B2	20070628			

PRIORITY APPLN. INFO.:

WO 1996-US18977	A	19961127
WO 1996-US20252	W	19961223
US 1999-319054	A2	19990526
WO 1999-US29792	A1	19991214
US 2000-621780	A2	20000721
CA 1996-2271889	A3	19961127
AU 1997-13382	A3	19961223
WO 1996-US20329	W	19961223
US 1998-112389P	P	19981215
US 1999-286818	A2	19990406
US 1999-308972	A2	19990527
US 1999-389211	A2	19990902
WO 2001-US22360	W	20010717
AU 2002-21302	A3	20020306

AB A method for producing a chewing gum with a controlled release of a bitterness inhibitor, as well as the chewing gum so produced, is obtained by phys. modifying the release properties of the bitterness inhibitor by coating and drying. The bitterness inhibitor is coated by encapsulation, partially coated by agglomeration, entrapped by absorption, or treated by multiple steps of encapsulation, agglomeration, and absorption. The coated bitterness inhibitor is preferably then co-dried and particle sized to produce a release-modified bitterness inhibitor for use in chewing gum. When incorporated into the chewing gum, these particles are adapted to produce a fast release or a delayed release when the gum is chewed. The preferred bitterness inhibitor is sodium gluconate.

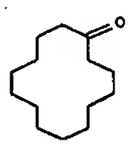
IT 117396-80-2D, Cyclotetradecenone, derivs.
RL: FFD (Food or feed use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(bitterness inhibitor; method of controlling release of bitterness inhibitors in chewing gum, and gum produced thereby)

RN 117396-80-2 CAPLUS

CN Cyclotetradecenone (9CI) (CA INDEX NAME)

CM 1

CRN 3603-99-4
CMF C14 H26 O



L28 ANSWER 2 OF 212 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:150485 CAPLUS Full-text
DOCUMENT NUMBER: 138:199984
TITLE: Cloning and characterization of Streptomyces lavendulae gene mcrA conferring resistance to DNA alkylating agents mitomycin C and use thereof in screening for antitumor agents
INVENTOR(S): Sherman, David H.; August, Paul R.; Flickinger, Michael C.
PATENT ASSIGNEE(S): Regents of the University of Minnesota, USA
SOURCE: U.S., 50 pp., Cont.-in-part of U.S. Ser. No. 133,963, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
US 6524812	B1	20030225	US 1996-624447	19960819	
WO 9509926	A1	19950413	WO 1994-US11279	19941006	<--
W: JP, US					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
US 6495348	B1	20021217	US 1999-266965	19990312	<--

PRIORITY APPLN. INFO.:

US 1993-133963	B2	19931007
WO 1994-US11279	W	19941006
US 1996-624447	A2	19960819

AB The invention provides genes encoding resistance to DNA bioreductive alkylating or cleaving agents and methods of identifying and using those genes. Specifically, gene mcrA conferring resistance to mitomycin C (MMC) is identified from cloned mcd locus, which is 3 open reading frames: (1) mcrA (formerly mcrA1), (2) mcrB (formerly mcrA2), and (3) mcrORF3 (formerly mcrAORF3). The purified gene mcrA protein is a 56 kDa protein detected on SDS-PAGE gel. Gene expression of mcrA is induced by low levels of MMC shown from a test using a series of mitomycins and related compds. In terms of the function mechanism, McrA protein acts in vivo by protecting S. lavendulae from adverse affects of MMC through maintaining the non-activated oxidative state of mol. Vectors for recombinant mcrA expression and their use in drug screening are also provided.

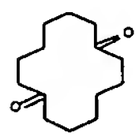
IT 152637-02-0
RL: MSC (Miscellaneous)
(genes encoding resistance to DNA alkylating agents)

RN 152637-02-0 CAPLUS

CN Cyclotetradecatetraenediyne-1,8-dione, bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

CM 1

CRN 152637-01-9
CMF C22 H40 O2
CCI IDS



z (D1-Bu-t)

REFERENCE COUNT: 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 3 OF 212 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:944465 CAPLUS Full-text
DOCUMENT NUMBER: 138:28944
TITLE: Skin-care products containing melanin inhibitors
INVENTOR(S): Matsuda, Hiroyuki; Yamamoto, Kenichi; Tamai, Eiko; Hagiwara, Toshimitsu; Yagi, Misao; Watanabe, Sinya; Kumamoto, Hiroyasu
PATENT ASSIGNEE(S): Takasago International Corporation, Japan
SOURCE: Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
EP 1264594	A2	20021211	EP 2002-291413	20020607	<--
EP 1264594	A3	20030305			
EP 1264594	B1	20061129			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2002363071	A	20021218	JP 2001-173655	20010608	<--
JP 2003119128	A	20030423	JP 2001-315378	20011012	
US 2003049213	A1	20030313	US 2002-164702	20020610	
US 6759557	B2	20040706			

PRIORITY APPLN. INFO.:

JP 2001-173655	A	20010608
JP 2001-315378	A	20011012

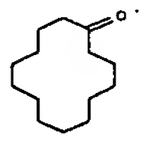
OTHER SOURCE(S): MARPAT 138:28944

AB The invention relates to a melanin synthesis inhibitor composition containing at least one macrocyclic compound such as cyclotetradecanone, cyclopentadecanone, 4-cyclopentadecenone. Thus, a cosmetic lotion was prepared from 2 phases; the oil phase contained 5-cyclohexadecenol 0.01, EtOH 20.0, hydrogenated ethoxylated castor oil 0.05, Me p-hydroxybenzoate 0.1, and perfume 0.1%; the aqueous phase comprised glycerin 10.0, 1,3-butylene glycol 5.0, and water qs to 100%. The 2 phases were mixed to give a cosmetic lotion which had a skin-lightening effect and good storage stability. The effectiveness of this compound in inhibiting melanin synthesis was demonstrated. The prepns. of the compds. of the invention, e..g, cycloalkanones, cycloalkenols, are given.

IT 3603-99-4, Cyclotetradecanone
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(skin-care products containing melanin inhibitors)

RN 3603-99-4 CAPLUS

CN Cyclotetradecanone (CA INDEX NAME)



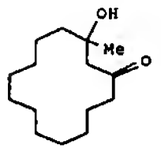
L28 ANSWER 4 OF 212 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:742335 CAPLUS Full-text
DOCUMENT NUMBER: 138:187448
TITLE: Direct, practical, and powerful crossed aldol additions between ketones and ketones or aldehydes utilizing environmentally benign TiCl4-Bu3N reagent
AUTHOR(S): Tanabe, Yoo; Matsumoto, Noriaki; Higashi, Takahiro; Misaki, Tomonori; Itoh, Tomotaka; Yamamoto, Misako; Mitarai, Kumi; Nishii, Yoshinori
CORPORATE SOURCE: School of Science and Technology, Department of Chemistry, Kwansei Gakuin University, Hyogo, 669-1337, Japan
SOURCE: Tetrahedron (2002), 58(41), 8269-8280
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:187448

AB An efficient TiCl4-Bu3N-(cat. TMSCl)-promoted aldol addition between ketones and ketones or aldehydes was performed. This environmentally benign method is advantageous from a green chemical viewpoint with regard to yield, substrates variation, reagent availability, and simple procedures. This method was applied to a short step formal synthesis of (R)-muscone, a natural macrocyclic musk.

IT 499195-95-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(crossed aldol addns. between ketones and ketones or aldehydes utilizing environmentally benign TiCl4-Bu3N reagent)

RN 499195-95-8 CAPLUS

CN Cyclotetradecanone, 3-hydroxy-3-methyl- (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 5 OF 212 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:671899 CAPLUS Full-text
DOCUMENT NUMBER: 137:201099

TITLE: Process for the preparation of macrocyclic ketones
INVENTOR(S): Frater, Georg; Nagel, Matthias
PATENT ASSIGNEE(S): Givaudan SA, Switz.
SOURCE: Eur. Pat. Appl., 26 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1236707	A1	20020904	EP 2001-103613	20010222 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
WO 2002068372	A1	20020906	WO 2002-EP1644	20020215 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002250956	A1	20020912	AU 2002-250956	20020215 <--
EP 1362023	A1	20031119	EP 2002-719851	20020215
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CN 1489566	A	20040414	CN 2002-804463	20020215
JP 2004527497	T	20040909	JP 2002-567888	20020215
CN 1824636	A	20060830	CN 2006-10068278	20020215
IN 2003CN01294	A	20051125	IN 2003-CN1294	20030819
US 2004082816	A1	20040429	US 2003-469177	20030822
US 6951964	B2	20051004		

PRIORITY APPLN. INFO.:	EP 2001-103613	A	20010222
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	WO 2002-EP1644	W	20020215

OTHER SOURCE(S): CASREACT 137:201099; MARPAT 137:201099
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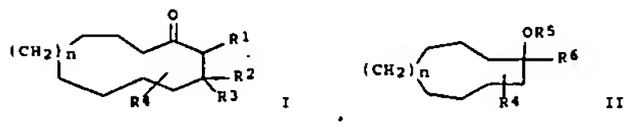
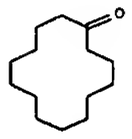
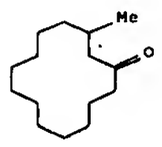


AB Macrocyclic ketones I [n = 0-7; R1-R4 = H, alkyl; R1R2 = bond] are prepared by heating a macrocyclic alc. II [R5 = H, trialkylsilyl; R6 = CR1:CR2R3, C.tplbond.CR3] at 500-700° and removing the trialkylsilyl group if present. II are prepared by complexing a macrocyclic ketone with CeCl3 and treatment with an organometallic reagent. Thus, cyclododecanone was complexed with CeCl3 and treated with H2C:CHMgBr to give 1-vinyl-1-cyclododecanol which was heated at 660±10° and 4-6 mbar to give 88% cyclotetradecanone.
IT 3603-99-4P, Cyclotetradecanone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the preparation of macrocyclic ketones)
RN 3603-99-4 CAPLUS

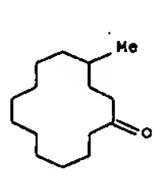
CN Cyclotetradecanone (CA INDEX NAME)



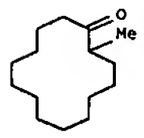
IT 22460-47-5P, 3-Methylcyclotetradecanone 36152-13-3P, 4-Methylcyclotetradecanone 75311-77-2P, 2-Methylcyclotetradecanone 434312-84-2P, 3,3-Dimethylcyclotetradecanone 434312-87-5P, 2,3-Dimethylcyclotetradecanone 454174-52-8P, 4-Ethylcyclotetradecanone 454174-53-9P, 3,4-Dimethylcyclotetradecanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of macrocyclic ketones)
RN 22460-47-5 CAPLUS
CN Cyclotetradecanone, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



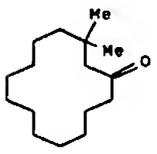
RN 36152-13-3 CAPLUS
CN Cyclotetradecanone, 4-methyl- (9CI) (CA INDEX NAME)



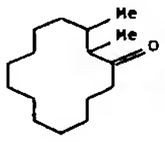
RN 75311-77-2 CAPLUS
CN Cyclotetradecanone, 2-methyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



RN 434312-84-2 CAPLUS
CN Cyclotetradecanone, 3,3-dimethyl- (CA INDEX NAME)



RN 434312-87-5 CAPLUS
CN Cyclotetradecanone, 2,3-dimethyl- (CA INDEX NAME)



RN 454174-52-8 CAPLUS
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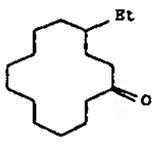
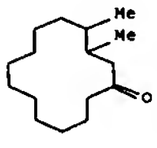


RN 454174-53-9 CAPLUS
CN Cyclotetradecanone, 3,4-dimethyl- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS

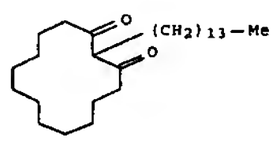
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 6 OF 212 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:582665 CAPLUS Full-text
DOCUMENT NUMBER: 137:124929
TITLE: Process for preparing higher primary alkanols
INVENTOR(S): Braier, Arnold; Rettig, Martin; Rey, Max
PATENT ASSIGNEE(S): Cilag A.-G., Switz.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002059101	A1	20020801	WO 2002-EP953	20020125 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1227087	A1	20020731	EP 2001-200275	20010126 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CA 2461450	A1	20020801	CA 2002-2461450	20020125 <--
AU 2002249150	A1	20020806	AU 2002-249150	20020125 <--
EP 1358170	A1	20031105	EP 2002-718061	20020125
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.:	EP 2001-200275	A	20010126
	WO 2002-EP953	W	20020125

OTHER SOURCE(S): CASREACT 137:124929; MARPAT 137:124929
AB The present invention concerns a process for preparing higher primary alkanols and in particular for preparing 1-octacosanol comprising a multistep process involving reacting cyclododecanone with a secondary amine, reacting the resulting 1-amino-1-cyclododecene with an activated alkanoic acid, subjecting the thus obtained 2-alkylcyclotetradecane-1,3-dione to a ring opening reaction and a Wolff-Kishner conversion, esterifying the thus obtained alkanoic acid with an alkanol and subsequently reducing the thus obtained ester to the desired higher primary alc. Thus, 1-octacosanol was prepared from cyclotetradecanone and palmitoyl chloride.
IT 117384-40-4P, 2-Tetradecyl-1,3-cyclotetradecanedione
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for preparing higher primary alkanols)
RN 117384-40-4 CAPLUS
CN 1,3-Cyclotetradecanedione, 2-tetradecyl- (CA INDEX NAME)

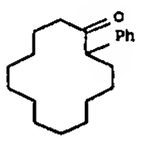


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 7 OF 212 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:517057 CAPLUS Full-text
DOCUMENT NUMBER: 137:201043
TITLE: Spin and Molecular Dynamics in Acyl-Containing Biradicals: Time-Resolved Electron Paramagnetic Resonance and Laser Flash Photolysis Study
AUTHOR(S): Tsentalovich, Yuri P.; Forbes, Malcolm D. E.; Morozova, Olga B.; Plotnikov, Igor A.; McCaffrey, Vanessa P.; Yurkovskaya, Alexandra V.
CORPORATE SOURCE: International Tomography Center, Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia
SOURCE: Journal of Physical Chemistry A (2002), 106(31), 7121-7129
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A combination of time-resolved ESR (TREPR) and laser flash photolysis (LFP) studies of flexible acyl-containing biradicals over a wide temperature range is reported. In contrast to previous reports, it is shown that the main channel of intersystem crossing in these biradicals is the electron spin relaxation of the acyl moiety rather than spin-orbit interaction in the biradical. This relaxation dets. the decay rate of the electron spin polarization at low temps. and the biradical lifetime at high temps. The relaxation mechanism is attributed to the spin-rotation interaction, associated with the rotation of the carbonyl group about the neighboring C-C bond axis. From a model simulation of the time profile of the spin-polarized TREPR signal based on the numerical solution of the stochastic Liouville equation of the spin d. matrix in frame of realistic model of biradical, the Arrhenius parameters for correlation times of spin rotation interaction and activation energies for mol. and spin dynamics were determined in two solvents, 2-propanol and hexane.

IT 101565-27-9, Cyclotetradecanone, 2-phenyl-
RL: RCT (Reactant); RACT (Reactant or reagent)
(CIDEP and transient optical absorption study of spin and mol. dynamics in acyl-containing biradicals)
RN 101565-27-9 CAPLUS
CN Cyclotetradecanone, 2-phenyl- (9CI) (CA INDEX NAME)



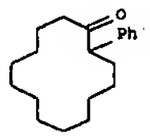
REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 8 OF 212 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:386458 CAPLUS Full-text
DOCUMENT NUMBER: 137:169193
TITLE: Spin relaxation in acyl radicals measured using spin correlated radical pair (SCRP) polarization in flexible biradicals
AUTHOR(S): Tsentalovich, Yuri P.; Forbes, Malcolm D. E.
CORPORATE SOURCE: International Tomography Center, Siberian Branch of

Russian Academy of Sciences, Novosibirsk, Russia
SOURCE: Molecular Physics (2002), 100(8), 1209-1213
CODEN: MOPHAM; ISSN: 0026-8976
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Time resolved ESR spectra and the decay kinetics of spin correlated radical pair (SCRP) polarization in an acyl-benzyl biradical were measured over a wide temperature range (180-274 K). The major mechanism of intersystem crossing in this biradical is the spin rotation induced relaxation of the acyl moiety, which is associated with the rotation of the carbonyl group about the neighboring CC bond axis. This relaxation dets. the decay rate of the polarization. The relaxation time is largely viscosity independent; it changes by a factor of less than two going from room temperature (60 ns) to 180 K (110 ns) in 2-propanol.

IT 101565-27-9, Cyclotetradecanone, 2-phenyl-
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(spin relaxation in acyl radicals measured using spin-correlated radical pair polarization in flexible biradicals)
RN 101565-27-9 CAPLUS
CN Cyclotetradecanone, 2-phenyl- (9CI) (CA INDEX NAME)



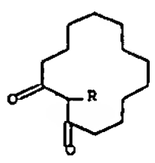
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

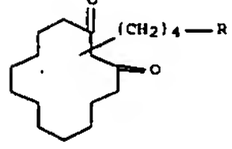
L28 ANSWER 9 OF 212 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:249008 CAPLUS Full-text
DOCUMENT NUMBER: 137:79311
TITLE: Synthesis and characterization of polyethylene-like polyurethanes derived from long-chain, aliphatic α,ω-diols
AUTHOR(S): McKiernan, Robin L.; Gido, Samuel P.; Penelle, Jacques
CORPORATE SOURCE: Department of Polymer Science and Engineering, University of Massachusetts, Amherst, MA, 01003-4530, USA
SOURCE: Polymer (2002), 43(10), 3007-3017
CODEN: POLMAG; ISSN: 0032-3861
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Long-chain aliphatic α,ω-diols containing up to 32 consecutive methylene groups were synthesized by several methods and characterized. 1,22-Docosanediol and 1,32-dotriacontanediol both exhibited a solid-solid phase transition before melting. The α,ω-diols HO(CH2)mOH, where m = 12, 22, or 32, were reacted in the melt with much shorter aliphatic α,ω-diisocyanates OCN(CH2)nNCO, where n = 4, 6, 8, or 12, producing a series of linear, aliphatic, and increasingly polyethylene-like m,n-polyurethanes. Characterization (by DSC, TGA, and SAXS) of the m,n-polyurethane series showed that when the aliphatic segments were increased, and the hydrogen-bonding densities thus decreased, the polymers displayed phys. and thermal properties (for example, solubility and melting temperature) typical of polyethylene.

IT 5009-06-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(intermediate; in synthesis of long-chain aliphatic α,ω-diols for preparation of polyethylene-like polyurethanes)
RN 5009-06-3 CAPLUS
CN 1,3-Cyclotetradecanedione, 2,2'-(1,4-butanediyl)bis- (9CI) (CA INDEX NAME)





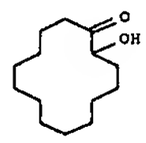
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 10 OF 212 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:203141 CAPLUS Full-text
DOCUMENT NUMBER: 137:20166
TITLE: A facile electrochemical approach for the synthesis of macrocyclic alkanones
AUTHOR(S): Singh, Arpita; Singhal, Nishi; Agrawal, Hemlata; Yadav, Ashok K.
CORPORATE SOURCE: Department of Chemistry, University of Rajasthan, Jaipur, 302 004, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2002), 41B(2), 423-426
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:20166

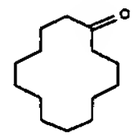
AB The synthesis of macrocyclic alkanones, viz. cyclotetradecanone, cyclohexadecanone, cyclooctadecanone, cyclopentadecanone and cycloheptadecanone have been carried out by using Kolbe sym./unsym. dimerization followed by cyclization in Na-xylene and subsequent reduction with Zn-HCl in 70-80% yield. The products of anodic cross coupling have been separated by column chromatog. over silica gel (60-120 mesh) by eluting with benzene-methanol (95:5). An effort has been made to optimize the electrochem. step by investigating the effect of different parameters, viz. degree of partial neutralization, c.d. and electrode material. The products have been characterized by elemental analyses and IR and 1H NMR spectral data.

IT 54561-32-9P, 2-Hydroxycyclotetradecanone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of macrocyclic cycloalkanones via electrochem. Kolbe reaction of alkanedioic acid esters)
RN 54561-32-9 CAPLUS

CN Cyclotetradecanone, 2-hydroxy- (CA INDEX NAME)



IT 3603-99-4P, Cyclotetradecanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of macrocyclic cycloalkanones via electrochem. Kolbe reaction of alkanedioic acid esters)
RN 3603-99-4 CAPLUS
CN Cyclotetradecanone (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	57.06	953.57
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-7.80	-10.14

FILE 'REGISTRY' ENTERED AT 13:50:03 ON 08 NOV 2007
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STRUCTURE FILE UPDATES: 7 NOV 2007 HIGHEST RN 952647-77-7
DICTIONARY FILE UPDATES: 7 NOV 2007 HIGHEST RN 952647-77-7

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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L4             SCREEN 1139
L5           3 S L2 AND L4 AND L1 SSS SAM
L6             SCREEN 1138
L7           0 S L2 AND L4 AND L6 AND L1 SSS SAM
L8             STRUCTURE UPLOADED
L9           0 S L8 SSS SAM
L10          0 S L4 AND L8 SSS SAM
L11          0 S L4 AND L6 AND L8 SSS SAM
L12       5360 S C14/ESS
L13          0 S L8 SSS SAM SUB=L12
L14          5 S L8 SSS FULL SUB=L12
L15      58806 S C12/ESS OR C13/ESS OR                C14/ESS OR C15/ESS OR C
L16      53391 S OC11/ESS OR OC12/ESS OR                OC13/ESS OR OC14/ESS
L17        417 S SC11/ESS OR SC12/ESS OR                SC13/ESS OR SC14/ESS
L18       3857 S NC11/ESS OR NC12/ESS OR                NC13/ESS OR NC14/ESS
L19     131063 S L15 OR L16 OR L17 OR 118
L20          5 S SSS FULL L8 SUB=L19

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L24            SCREEN 1139
L25       7017 S L24  SUB=L23 FULL
L26        180 S SSS FULL L1 SUB=L19

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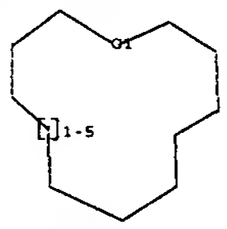

G1 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

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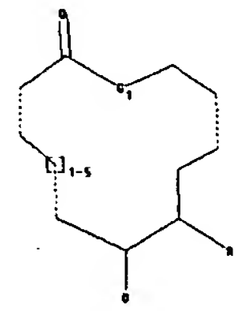

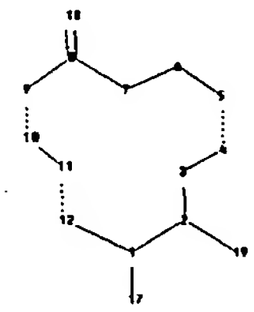

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chain nodes :
17  18  19
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12
chain bonds :
1-17  2-19  8-18
ring bonds :
1-2  1-12  2-3  3-4  4-5  5-6  6-7  7-8  8-9  9-10  10-11  11-12
exact/norm bonds :
1-2  1-12  1-17  2-3  2-19  3-4  4-5  5-6  6-7  7-8  8-9  8-18  9-10  10-11  11-12

isolated ring systems :
containing 1 :
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G1:C,O,S,N


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Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  17:CLASS  18:CLASS  19:CLASS
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L29 STRUCTURE UPLOADED

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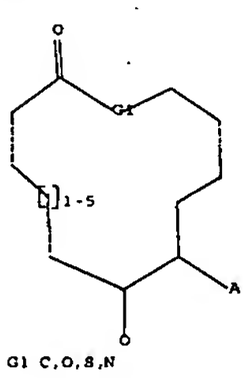

G1 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

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FULL SUBSET SCREEN SEARCH COMPLETED -     57167 TO ITERATE

100.0% PROCESSED     57167 ITERATIONS                                 34 ANSWERS
SEARCH TIME: 00.00.01

L30           34 SEA SUB=L19 SSS FUL L29

=> d scan

L30  34 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   Oxacyclotetradeca-7,12-dien-2-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]o
     xy]-9-methoxy-11,13-dimethyl-14-(1-methylethyl)-, (7E,9S,10S,11R,12Z,14S)-
MF   C25 H46 O4 Si

Absolute stereochemistry.
Double bond geometry as shown.
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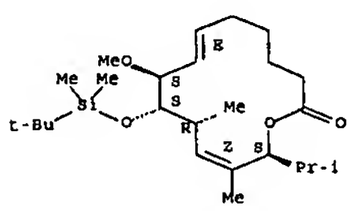


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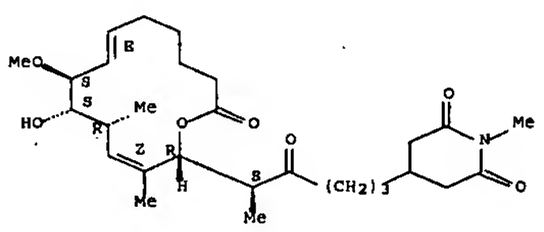
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L30  34 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E)-6-hydroxy-7-methoxy-
     3,5-dimethyl-14-oxooxacyclotetradeca-3,8-dien-2-yl]-4-oxohexyl]-1-methyl-
MF   C28 H43 N O7

Absolute stereochemistry.
Double bond geometry as shown.
```

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L30  34 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-,
     (2R,3Z,5R,6S,7S,8E,12E)-2-[(1S)-5-(2,6-dioxo-4-piperidinyl)-1-methyl-2-
     oxopentyl]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-6-
     yl ester, (αS)-
MF   C37 H46 F3 N O9

Absolute stereochemistry.  Rotation (+).
Double bond geometry as shown.
```

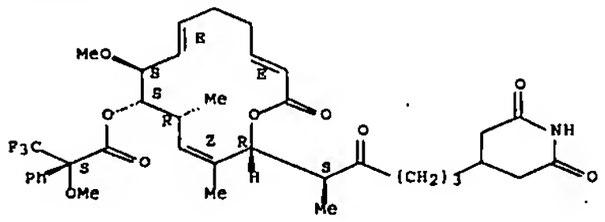

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-10.14

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=> s l30
L31 32 L30

=> s l31 and py<2003
22908272 PY<2003
L32 10 L31 AND PY<2003

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L32 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:971943 CAPLUS Full-text
DOCUMENT NUMBER: 138:271829
TITLE: Synthetic studies on the dienophile unit of methyl isosartortuoate. Part 2: SmI2-mediated 14-membered carbocyclization
AUTHOR(S): Hong, Zhangyong; Xu, Xingxiang
CORPORATE SOURCE: Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Tetrahedron Letters (2002), Volume Date 2003, 44(3), 489-491
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:271829
GI

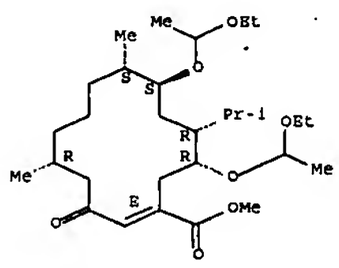
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The dienophile unit, I, of Me isosartortuoate has been synthesized. The 14-membered carbocycle was constructed via a SmI2-mediated intramol. Reformatskii reaction of formyl ester II. The introduction of the oxo group at the γ-position of the α,β-unsatd. ester was achieved via rearrangement of β,γ-epoxy ester III.

IT 503446-48-8P 503446-51-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dienophile unit of Me isosartortuoate via SmI2-mediated intramol. Reformatskii-cyclization of formyl ester and rearrangement of β,γ-epoxy ester)

RN 503446-48-8 CAPLUS
CN 1-Cyclotetradecene-1-carboxylic acid, 10,13-bis(1-ethoxyethoxy)-5,9-dimethyl-12-(1-methylethyl)-3-oxo-, methyl ester, (1E,5R,9S,10S,12R,13R)-(CA INDEX NAME)

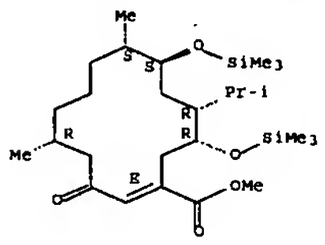
Absolute stereochemistry.
Double bond geometry as shown.



RN 503446-51-3 CAPLUS
CN 1-Cyclotetradecene-1-carboxylic acid, 5,9-dimethyl-12-(1-methylethyl)-3-oxo-10,13-bis[(trimethylsilyl)oxy]-, methyl ester, (1E,5R,9S,10S,12R,13R)-(CA INDEX NAME)

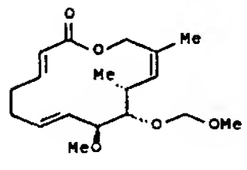
Absolute stereochemistry.

Double bond geometry as shown.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:862418 CAPLUS Full-text
DOCUMENT NUMBER: 138:153349
TITLE: Synthesis of the macrolide core of migrastatin
AUTHOR(S): Gaul, Christoph; Danishefsky, Samuel J.
CORPORATE SOURCE: Laboratory for Bioorganic Chemistry, Sloan-Kettering Institute for Cancer Research, New York, NY, 10021, USA
SOURCE: Tetrahedron Letters (2002), 43(50), 9039-9042
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:153349
GI



I

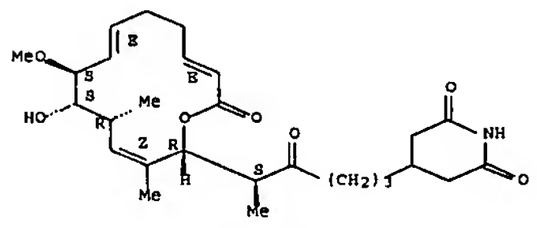
AB A concise and efficient synthesis of the macrolactone core I of migrastatin, a new natural product with potent anticancer properties, has been achieved. The key features of our synthetic strategy encompass a Lewis acid catalyzed diene aldehyde condensation (LACDAC) to install the three contiguous stereocenters and the trisubstituted (Z)-double bond of migrastatin, and a (E)-selective ring-closing metathesis (RCM) to construct the macrocycle.

IT 314245-65-3P, Migrastatin
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of the macrolactone core of migrastatin utilizing lewis acid catalyzed diene aldehyde condensation and ring-closing metathesis)

RN 314245-65-3 CAPLUS
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-

oxohexyl]- (CA INDEX NAME)

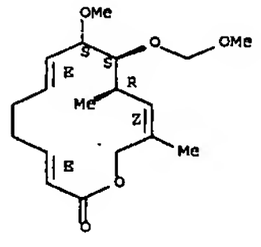
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT 494834-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of the macrolactone core of migrastatin utilizing lewis acid catalyzed diene aldehyde condensation and ring-closing metathesis)

RN 494834-82-1 CAPLUS
CN Oxacyclotetradeca-3,7,12-trien-2-one, 9-methoxy-10-(methoxymethoxy)-11,13-dimethyl-, (3E,7E,9S,10S,11R,12Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:650739 CAPLUS Full-text
DOCUMENT NUMBER: 137:184573
TITLE: Fermentation and purification of migrastatin and analog
INVENTOR(S): Khosla, Chaitan; Licari, Peter; Carney, John
PATENT ASSIGNEE(S): Kosan Biosciences, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 7 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 2002119937	A1	20020829	US 2001-932167	20010817 <--
US 6750047	B2	20040615		
US 2004209336	A1	20041021	US 2004-838895	20040503

PRIORITY APPLN. INFO.: US 2000-226595P P 20000821
US 2001-932167 A3 20010817

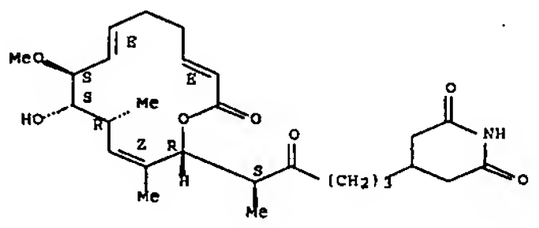
AB Migrastatin and a migrastatin analog can be produced by fermentation of Streptomyces platensis NRRL 18993 and used in pharmaceutical formulations to treat cancer and/or inhibit metastasis of cancer cells.

IT 314245-65-3P, Migrastatin
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(fermentation and purification of migrastatin and analog)

RN 314245-65-3 CAPLUS

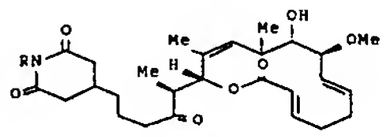
CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:340580 CAPLUS Full-text
DOCUMENT NUMBER: 137:154778
TITLE: Absolute configuration of migrastatin, a novel 14-membered ring macrolide. Comments.
AUTHOR(S): Nakamura, Hiraku
CORPORATE SOURCE: Japan
SOURCE: Journal of Antibiotics (2002), 55(4), 442-444
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:154778
GI



I

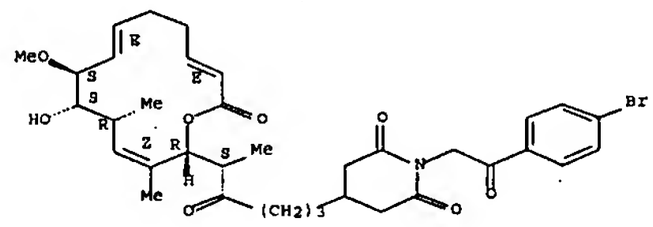
AB The X-ray crystallog. anal. of N-p-bromophenacylmigrastatin I (R = CH2CO-p-C6H4-Br) led the establishment of absolute configuration of migrastatin I (R = H), a novel 14-membered ring macrolide, isolated from a culture broth of Streptomyces sp. MK929-43F1.

IT 445489-47-4P, (+)-N-p-Bromophenacylmigrastatin
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; determination of absolute configuration of migrastatin via X-ray crystallog. anal. of N-p-bromophenacylmigrastatin)

RN 445489-47-4 CAPLUS

CN 2,6-Piperidinedione, 1-[2-(4-bromophenyl)-2-oxoethyl]-4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

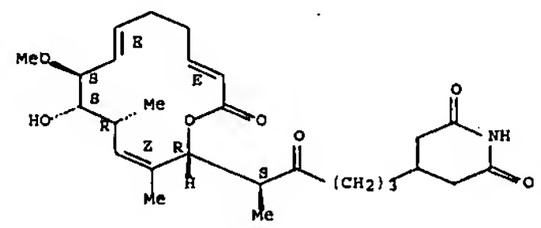


IT 314245-65-3
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(determination of absolute configuration of migrastatin via X-ray crystallog. anal. of N-p-bromophenacylmigrastatin)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



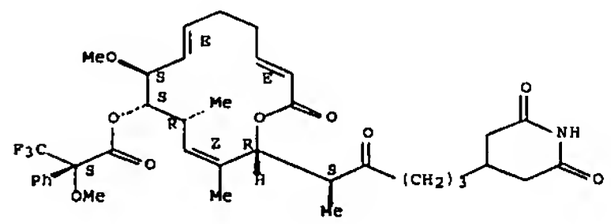
IT 444787-82-0P 444787-83-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(determination of absolute configuration of migrastatin via X-ray crystallog. anal.

of N-p-bromophenacylmigrastatin)

RN 444787-82-0 CAPLUS

CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, (2R,3Z,5R,6S,7S,8E,12E)-2-[(1S)-5-(2,6-dioxo-4-piperidinyl)-1-methyl-2-oxopentyl]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-6-yl ester, (αS)- (CA INDEX NAME)

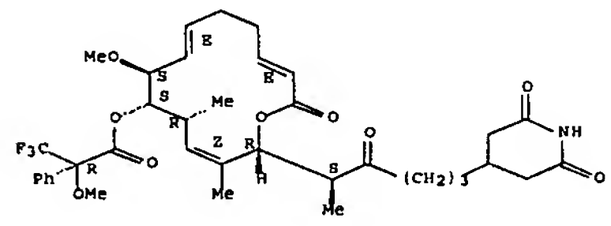
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 444787-83-1 CAPLUS

CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, (2R,3Z,5R,6S,7S,8E,12E)-2-[(1S)-5-(2,6-dioxo-4-piperidinyl)-1-methyl-2-oxopentyl]-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-6-yl ester, (αR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:203151 CAPLUS Full-text
DOCUMENT NUMBER: 136:339536
TITLE: Migrastatin and a new compound, isomigrastatin, from Streptomyces platensis
AUTHOR(S): Woo, Elaine J.; Starks, Courtney M.; Carney, John R.; Arslanian, Robert; Cadapan, Lawrence; Zavala, Stefan; Licari, Peter
CORPORATE SOURCE: Kosan Biosciences, Inc., Hayward, CA, 94545, USA
SOURCE: Journal of Antibiotics (2002), 55(2), 141-146

CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:339536

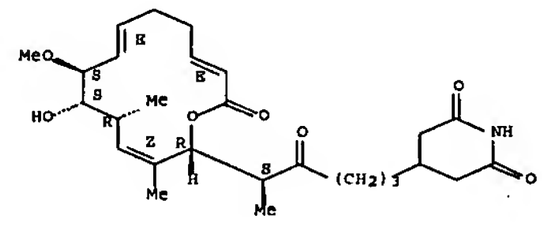
AB Streptomyces platensis (strain NRRL 18993), a producer of dorrigocins, was shown to produce migrastatin, a cyclic congener of dorrigocin A previously reported from a different organism. Addnl. a new compound isomeric to migrastatin, isomigrastatin, was also isolated and its structure was determined to be a cyclic form of dorrigocin B. Both compds. were fully characterized from MS and NMR data. Product titers of both were improved by the addition of XAD-16 resin to the fermentation medium.

IT 314245-65-3P, Migrastatin
RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(migrastatin and its isomer isomigrastatin from Streptomyces platensis fermentation)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:11968 CAPLUS Full-text
DOCUMENT NUMBER: 136:226436
TITLE: Migrastatin, a novel 14-membered ring macrolide, inhibits anchorage-independent growth of human small cell lung carcinoma Ms-1 cells
AUTHOR(S): Takemoto, Yasushi; Nakae, Koichi; Kawatani, Makoto; Takahashi, Yoshikazu; Naganawa, Hiroshi; Imoto, Masaya
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Science and Technology, Keio University, Yokohama, 223-8522, Japan
SOURCE: Journal of Antibiotics (2001), 54(12), 1104-1107
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effects of teleocidin-free migrastatin on tumor cell migration and on the growth of several types of tumor cells were reported. The original migrastatin contained about 0.1% teleocidin-related compds. Migrastatin inhibited migration of EC17 cells with an

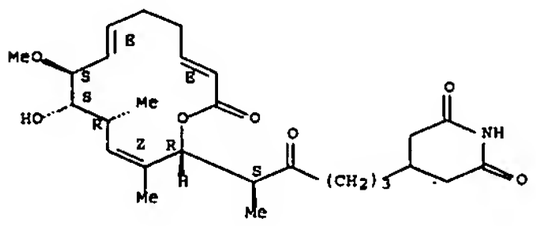
IC50 value of approx. 10μg/mL, but it inhibited cell proliferation of EC17 cells with an IC50 value of 82μg/mL, and it failed to induce cell death in EC17 cells up to 100 μg/mL. These results showed that the inhibited migration of EC17 cells by migrastatin should not be due to the inhibition of cell proliferation or induction cell death by the drug. Migrastatin did not considerably reduced the growth rate up to 30μg/mL, and 100μg/mL of migrastatin induced cell death as evaluated by trypan blue dye exclusion assay. It reduced the anchorage-independent growth ability of Ms-1 cells. The growth rate of Ms-1 cells under anchorage-independent condition was lower than that under anchorage-dependent condition.

IT 314245-65-?, Migrastatin
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(migrastatin inhibits anchorage-independent growth of human small cell lung carcinoma Ms-1 cells)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

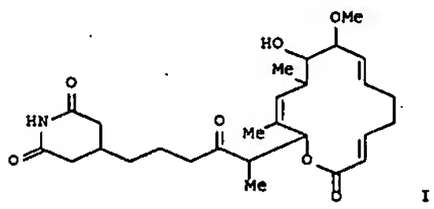
L32 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:472958 CAPLUS Full-text
DOCUMENT NUMBER: 135:45279
TITLE: Migrastatin, process for producing the same and medicinal compositions
INVENTOR(S): Takeuchi, Tomio; Sawa, Tsutomu; Hamada, Masa; Naganawa, Hiroshi; Takahashi, Yoshigazu; Imoto, Masaya; Nakae, Kouichi
PATENT ASSIGNEE(S): Zaidan Hojin Biseibutsu Kagaku Kenkyu Kai, Japan
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046451	A1	20010628	WO 2000-JP9147	20001222 <--

W: AU, CA, CN, JP, US
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR

PRIORITY APPLN. INFO.: JP 1999-364316 A 19991222

GI



I

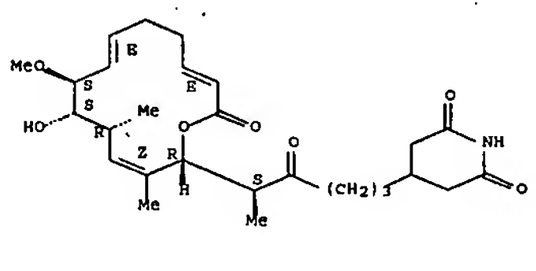
AB Migrastatin (I) is manufactured by culturing Streptomyces sp. MK929-43F1. Migrastatin has an anticancer activity against various human cancers or tumor cells, a cell motility inhibitory activity, and an angiogenesis inhibitory activity on vascular endothelial cells. Shake-culture of Streptomyces and purification of I by filtration, solvent extraction, and chromatog. was shown.

IT 314245-65-3P, Migrastatin
RL: BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Migrastatin, process for producing the same and medicinal compns.)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

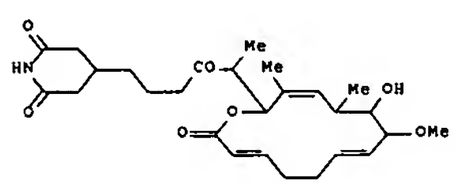
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:780072 CAPLUS Full-text
DOCUMENT NUMBER: 134:71413
TITLE: Migrastatin, a novel 14-membered lactone from Streptomyces sp. MK929-43F1
AUTHOR(S): Nakae, Koichi; Yoshimoto, Yuya; Ueda, Minoru; Sawa, Tsutomu; Takahashi, Yoshikazu; Naganawa, Hiroshi; Takeuchi, Tomio; Imoto, Masaya
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Science

and Technology, Keio University, Yokohama, 223, Japan
SOURCE: Journal of Antibiotics (2000), 53(10), 1228-1230
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

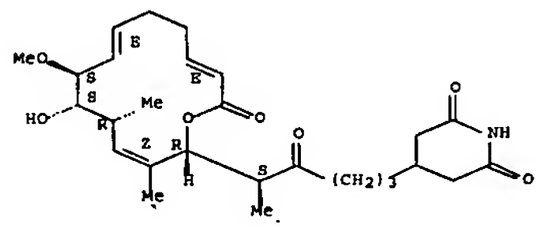
AB The mol. structure and olefinic bond geometry of migrastatin (I), a novel 14-membered lactone from Streptomyces sp. MK929-43F1, was determined by spectral means.

IT 314245-65-3, Migrastatin
RL: PRP (Properties)
(mol. structure of migrastatin, a novel 14-membered lactone previously isolated from Streptomyces sp. MK929-43F1)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

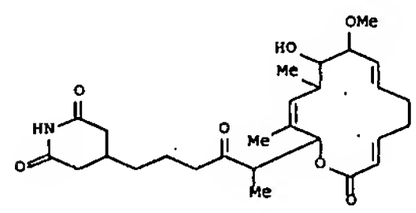
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:780057 CAPLUS Full-text
DOCUMENT NUMBER: 134:68523
TITLE: Migrastatin, a new inhibitor of tumor cell migration from Streptomyces sp. MK929-43F1. Taxonomy, fermentation, isolation and biological activities
AUTHOR(S): Nakae, Koichi; Yoshimoto, Yuya; Sawa, Tsutomu; Homma, Yoshiko; Hamada, Masa; Takeuchi, Tomio; Imoto, Masaya
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Science

and Technology, Keio University, Yokohama, 223-8522, Japan
SOURCE: Journal of Antibiotics (2000), 53(10), 1130-1136
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

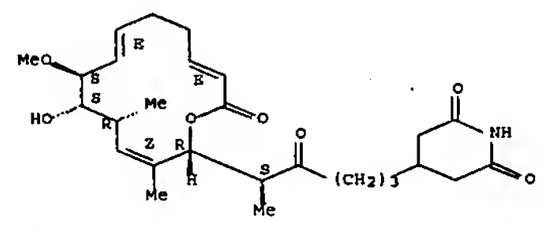
AB A new compound, migrastatin (I), was isolated from a cultured broth of Streptomyces sp. MK929-43F1, as an inhibitor of tumor cell migration. It was purified by column chromatogs. on silica gel and Sephadex LH-20 and HPLC. I has the mol. formula of C27H39NO7 consisting of 14-membered macrolide and glutarimide moiety. It inhibited spontaneous migration of human esophageal cancer EC17 cells. Migration inhibitory activity of I was not dependent on cytotoxicity or inhibition of protein synthesis.

IT 314245-65-3P, Migrastatin
RL: BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(migrastatin is a new inhibitor of tumor cell migration from Streptomyces MK929-43F1)

RN 314245-65-3 CAPLUS

CN 2,6-Piperidinedione, 4-[(5S)-5-[(2R,3Z,5R,6S,7S,8E,12E)-6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl]-4-oxohexyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:758793 CAPLUS Full-text
DOCUMENT NUMBER: 123:167722
TITLE: Bone-absorption inhibitors manufacture with Streptomyces
INVENTOR(S): Isogai, Kazuhide; Kagamizono, Terumi; Shinyashiki, Keiko; Kawashima, Akira; Morimoto, Shigeo; Chin, Sosho; Ko, Junmo
PATENT ASSIGNEE(S): Taisho Pharma Co Ltd, Japan; Kotsuka Iyaku Kanrikyoku Shise
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07138257	A	19950530	JP 1993-286343	19931116 <--
PRIORITY APPLN. INFO.:			JP 1993-286343	19931116

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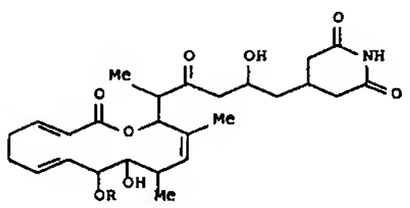
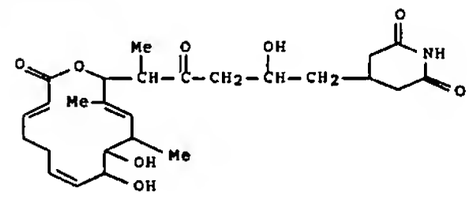


I

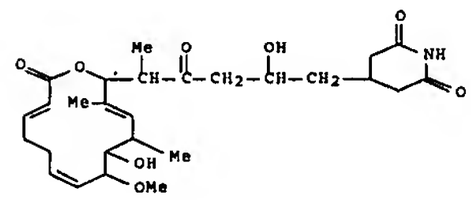
AB Bone-absorption inhibitors (I: R = H or Me) are manufactured by culturing Streptomyces hygroscopicus var. ossamyceticus TA-0247. Shake-culture of S. hygroscopicus var. ossamyceticus TA-0247 in a medium of oat meal, glucose, NaCl, etc., and recovery of I, i.e. BR-040 and BR-042, from fermentation broth by extraction and chromatogs. The IC50s of BR-040 and BR-042 against bone absorption were 50 μg/ml and 25, resp. The physiol. and morphol. characteristics of the microorganism were given.

IT 167503-59-5P, BR 040 167503-60-8P, BR 042
RL: BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(bone-absorption inhibitors manufacture with Streptomyces)

RN 167503-59-5 CAPLUS
CN 2,6-Piperidinedione, 4-[5-(6,7-dihydroxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl)-2-hydroxy-4-oxohexyl]- (9CI) (CA INDEX NAME)



RN 167503-60-8 CAPLUS
CN 2,6-Piperidinedione, 4-[2-hydroxy-5-(6-hydroxy-7-methoxy-3,5-dimethyl-14-oxooxacyclotetradeca-3,8,12-trien-2-yl)-4-oxohexyl]- (9CI) (CA INDEX NAME)



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Connection closed by remote host

Havlin, Robert

From: Schulwitz, Paul
Sent: Monday, November 05, 2007 3:21 PM
To: Havlin, Robert
Subject: Search results for 10/551,152

Examiner Havlin,

See the attached file for the results of your requested structure search:

20071105-1155115
2-str.rtf

There were over 25,000 compounds and references for the proppsed structure. I displayed 27 references for compounds hit in the structure search that are also associated with the indexing of the pre grant pub. for the instant application.
I only displayed a sample of the results for the broad structure search.
Please review the results and get back to me if you need a revised search to be run.

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Technical Information Specialist
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DP to

10/551,158

11/663,580